



Modellering af stoftransport i opsprækket kalk

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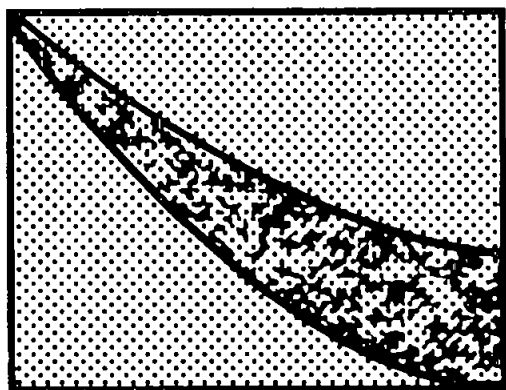
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**MODELLERING AF STOFTRANSPORT
I OPSPRÆKKET KALK**

RAPPORT M3 DECEMBER 1992

LOSSEPLADSPROJEKTET

FORORD

Rapporten beskriver en modelanalyse af et tracerforsøg udført i en opsprækket kalkbjergart ved en lokalitet nær Karlstrup. Feltundersøgelserne er udført inden for rammerne af Lossepladsprojektets Projekt H9, og disse er afrapporteret selvstændigt. Modelanalysen er foretaget med SHE modellen, som inden for rammerne af nærværende projekt er udvidet til også at kunne simulere stoftransport i et dobbeltporøst medium.

Rapporten består af en kortfattet præsentation af de vigtigste resultater, og som bilag er inkluderet en artikel, hvor data og resultater er mere udførligt præsenteret og diskuteret.

Der rettes en tak til Dansk Hydraulisk Institut for velvillig assistance i forbindelse med opsætningen og tilpasningen af SHE til den undersøgte lokalitet og problemstilling.

SAMMENFATNING

Med henblik på at undersøge de hydrauliske og transportmæssige forhold i en opsprækket kalkbjergart er der foretaget prøvepumpning, separationsinjektionsforsøg og tracerforsøg ved en lokalitet nær Karlstrup. De indsamlede feltdata er tolket ved numeriske modelsimuleringer af vandstrømning og stofudbredelse i det undersøgte område. Som model er anvendt SHE-systemets tre-dimensionale grundvandsmodel, som i forbindelse med projektet er udvidet til også at kunne simulere stoftransport i en dobbeltporøs bjergart. Modelformuleringen er baseret på den antagelse, at vandstrømning og transport kun forekommer i sprækkesystemet, og at der ved diffusion kan udveksles stof med stillestående porevand i det primære matrixsystem.

Strømningsforholdene er beskrevet i et modelnet, som dækker et område på ca. 150 m \times 150 m med en horisontal og vertikal diskretisering på henholdsvis 4.0 m og 2.2 m. Af hensyn til computertiden er stoftransporten beskrevet i et mindre område med en finere diskretisering på 2.0 m i horisontal retning og 2.2 m i vertikal retning.

I modellen anvendes målte værdier for de indgående parametre i det omfang målinger er foretaget. For en række parametre har det imidlertid været nødvendigt at introducere værdier, som er bestemt ved at kalibrere mod målte potentialer og gennembrudskurver.

Det har ikke været muligt at tilpasse en enkelt-porøsitetsmodel til de observerede gennembrudskurver, hvor det antages, at stoftransporten udelukkende sker enten i sprækkerne eller i det primære poresystem. Derimod har det været muligt at opnå en tilfredsstillende beskrivelse af de målte data, hvis der introduceres to porøsitetsdomæner. Sprækkeporøsiteten er estimeret til 1.5%, hvilket er i god overensstemmelse med målingerne. Derimod er det nødvendigt at anvende en værdi for matrixporøsiteten (4%), som er væsentligt lavere end målinger udført på udtagne prøver (20-35%). Denne forskel kan imidlertid forklares fysisk ved, at kun en lille

del af matrixvoluminet er aktivt involveret i diffusionsprocessen. Den langsgående horisontale dispersivitet er kalibreret til 8.0 m, hvilket er højt i forhold til den værdi, som er fundet ved lossepladsen ved Vejen og også i relation til forsøgets beskedne horisontale udstrækning (25 m). Den forhøjede dispersivitetsværdi forklares ved en forøget spredningseffekt fra sprække-systemets heterogene opbygning både hvad angår sprækkediameter og -orientering.

Der er foretaget en række følsomhedsanalyser på udvalgte fysiske parametre. Stor følsomhed er konstateret for diffusionskoefficienten for udvekslingen mellem sprækker og matrix, men også porøsitetsværdierne for både sprækker og matrix og dispersiviteten har stor indvirkning på formen af gennembrudskurverne.

Den væsentlige konklusion fra modelundersøgelsen er, at stoftransport i opsprækkede bjergarter ikke kan beskrives ved hjælp af en traditionel enkeltporøsitetsmodel, men at det er nødvendigt at tage højde for de fysiske forskelle, som betinger stofspredning i dels det meget permeable sprækkesystem og dels i den primære, mindre permeable matrix.

ENGLISH SUMMARY

Brettmann, Kenneth and Jensen, Karsten Høgh, 1991: Transport modelling in fractured chalk. Lossepladsprojekt, Rapport M3.

A two-well tracer test was conducted in eastern Denmark, in which a short duration pulse of lithium chloride was injected into a recharge well and made to flow through a fractured chalk aquifer to a discharge well. The wells were 25 meters apart, and the concentration of lithium arriving at the discharge well was monitored at five vertical intervals in the well for a 21 day period. The observed breakthrough curves show a sharp breakthrough front, with an arrival time that is consistent with advective transport through the fractures in the chalk. The breakthrough curves also exhibit a long tail in the falling limb, suggesting the influence of a secondary transport mechanism such as adsorption or diffusion of lithium into the porous matrix. To better understand the transport processes involved, a three-dimensional finite-difference model for flow and transport was constructed on the basis of geological and hydraulic information. The model was developed as a dual-porosity continuum model, in which advection was assumed to occur only in the fractures and the water in the porous matrix was assumed to be static. The exchange of solute between the fractures (mobile phase) and the porous matrix (immobile phase) was assumed to occur as a diffusion process in response to the local concentration difference of solute between the two phases. Simulations from the dual-porosity model correctly reproduced the shape of the observed breakthrough curves, although some portions of the tail were not accurately represented. The model was also applied as a single-porosity model, in which no diffusion or adsorption of solute were assumed to occur. The simulations from the single-porosity model greatly overestimated the observed lithium concentrations, and showed very little tailing effect in the falling limb. The study shows, that based on the given tracer test, solute transport in a fractured chalk cannot be represented by a single-porosity approach, and hence when dealing with conta-

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1. INDLEDNING

Med henblik på at undersøge de hydrauliske og transportmæssige forhold i et kalkmagasin er der foretaget feltundersøgelser ved en lokalitet nær Karlstrup. Kalkbjergarter er karakteriseret ved en dobbeltporøs struktur omfattende et sprækkedomæne med en porøsitet af størrelsesordenen 0.1-2.0% af bjergartsvoluminet og et matrixdomæne med en porøsitet af størrelsesordenen 20-40%.

Da den hydrauliske ledningsevne i sprækkerne er flere størrelsesordener større end i den omgivende matrix, er vandtransporten i hovedsagen knyttet til sprækkedomænet. Opløste forurenende stoffer, som følger med grundvandet, føres med stor hastighed gennem sprækkesystemet som følge af den meget lille porøsitet. Samtidig hermed sker der en udveksling af stof ved diffusion mellem sprækker og matrix i samme øjeblik, der optræder koncentrationsforskelle mellem de to domæner, se f.eks. Freeze og Cherry (1979).

De indsamlede data har dannet grundlag for opstilling og kalibrering af en tre-dimensional numerisk vandstrømnings- og stoftransportmodel (SHE). Modellen er udbygget, således at både enkeltporøsitets- og dobbeltporøsitetssystemer kan simuleres.

2. GEOLOGI OG HYDROGEOLOGI

De geologiske og hydrogeologiske forhold samt tracerforsøget er undersøgt og udført af Danmarks Geologiske Undersøgelse inden for rammerne af projekt H9, og disse undersøgelser er rapporteret i en særskilt rapport (Jacobsen, 1991). Nedenfor gives et kort resumé af disse.

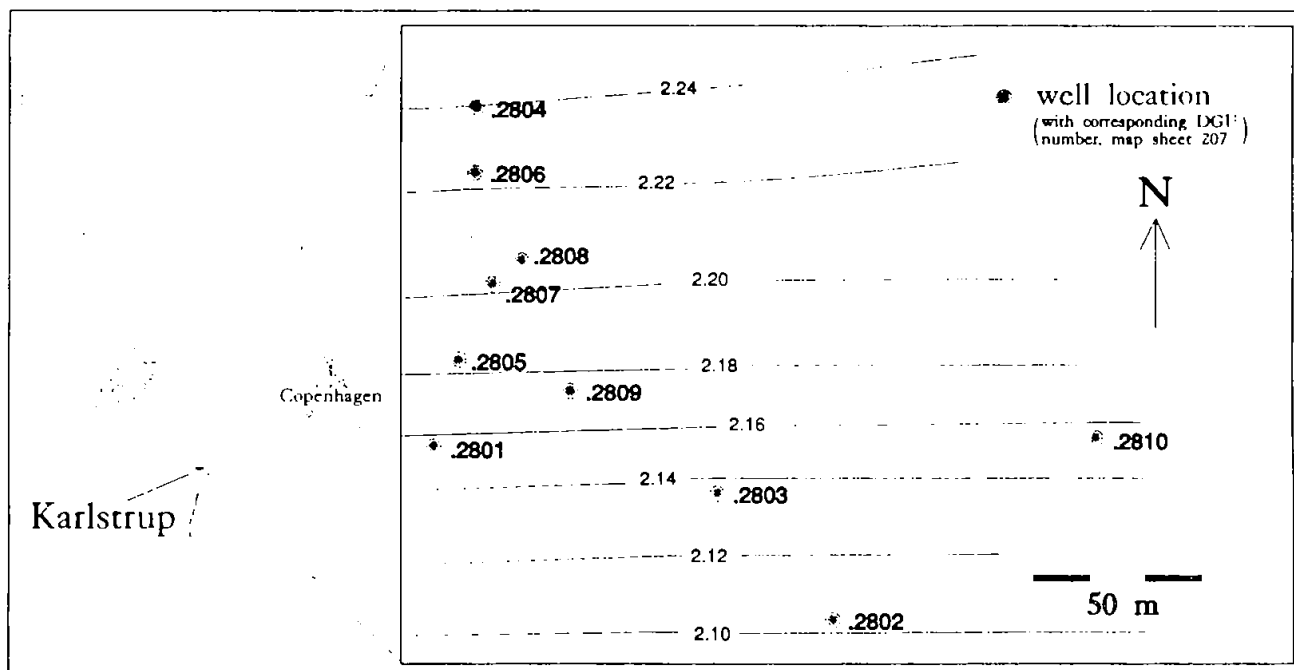
2.1 Geologiske forhold

Den undersøgte lokalitet ligger ved Karlstrup, 35 km syd for København. De dybere aflejringer i området består af bryozokalk opbygget i banker med indskudte lag af flint. Kalkbankerne har en del sprækker uden nogen dominerende retning. Sprækketætheden er størst i den øverste del af formationen og aftager hurtigt med dybden. Kalken er overlejret af et forholdsvist tyndt dæklag af moræneler, som har en tykkelse i intervallet 0 til 5 m indenfor undersøgelsesområdet.

2.2 Hydrogeologiske forhold

Selve undersøgelseområdet har en udstrækning på 80 × 120 m, og der er etableret i alt 10 boringer, som er filtersat til kote -20 m. Fig. 1 viser et kort over forsøgsfeltet med angivelse af boringerne placering, og endvidere er der vist et potentialkort for forholdene før forsøgenes udførelse.

Der er foretaget to prøvepumpninger samt udført Separations Injektions Test (SIT) i alle boringer med henblik på at bestemme vertikale fordelinger af hydraulisk ledningsevne. Disse undersøgelser har vist, at størst ledningsevne forekommer i de øverste 10 m af kalkformationen, hvor sprækketætheden er størst. I dette interval er den hydrauliske ledningsevne bestemt til 50-100 m/dag. Ud fra SIT forsøgene vurderes, at 95% af vandstrømningen foregår i dette interval. I den nedre del af kalken er sprækketætheden meget mindre, og den hydrauliske ledningsevne er her bestemt til ca. 5 m/dag.



Figur 1. Forsøgsfelt med placering af boringer samt potential-kort.

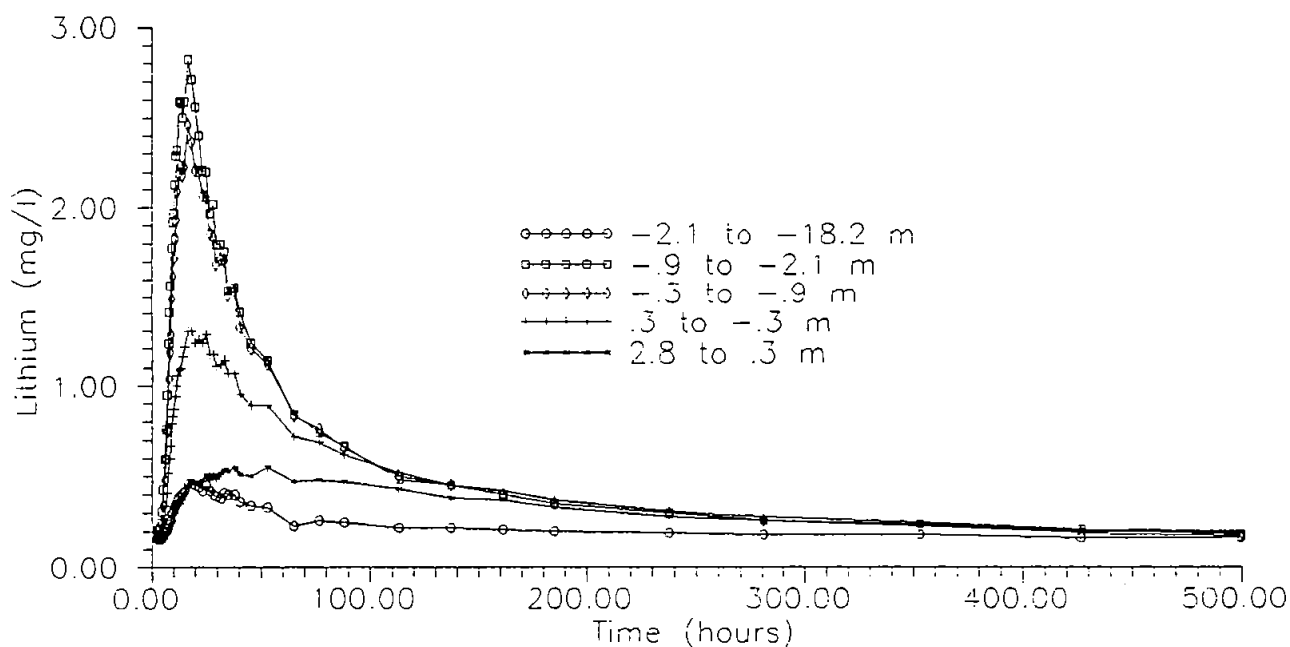
Sprækkeporøsiten i det øverste interval er ud fra kortvarige prøvepumpninger bestemt til ca 1.5% og matrixporøsiteten er målt til 20-30% på uforstyrrede sedimentprøver.

I størstedelen af undersøgelsesområdet er grundvandsspejlet frit, og kun i den sydlige del af området er der tale om artesiske forhold.

3. TRACERFORSØG

Der blev udført to sporstofforsøg i området ved at separationsinjicere sporstof i form af lithium (LiCl) i et 20% strømningspartiale med samtidig injektion af oppumpet grundvand over og under. I en nedstrøms beliggende boring blev der separationspumpet fra fem intervaller, som hver repræsenterede et 20% strømningspartiale bestemt ved SIT, Jacobsen (1991). Der blev udtaget vandprøver fra de fem pumper med jævne mellemrum for at bestemme den vertikale koncentrationsfordeling af sporstoffet i observationsboringen.

Det var hensigten at tilføre sporstoffet over et velafgrænset interval i injektionsboringen uden at anvende packere. Imidlertid skete der en vis opblanding over dybden, således at sporstoffet i realiteten blev injiceret over dybden med varierende koncentration. Denne fordeling blev målt med ledningsevнемåler. Der er kun foretaget modelberegninger for det andet forsøg, som vurderes at være behæftet med mindst usikkerhed. Gennembrudskurver for dette forsøg er illustreret i Fig. 2.



Figur 2. Observerede gennembrudskurver for lithium i fem dybder i boring 9.

Af kurverne fremgår, at de højeste koncentrationer forekommer i intervallet fra 0 - -2 m, hvilket svarer til det interval, hvor størstedelen af lithium blev injiceret. Gennembrudskurverne er asymmetriske og karakteriseret ved et hurtigt gennembrud og langsom aftagen, hvilket antyder, at transporten foregår i et opsprækket system.

4. NUMERISK MODEL OG MODELSIMULERING

Med henblik på at etablere en sammenhængende beskrivelse af strømnings- og transportforhold i det undersøgte område er der opstillet en tre-dimensional numerisk model med udgangspunkt i SHE-systemets grundvandsmodel (Ammertorp & Refsgaard, 1991). Modellen løser strømningsligningen (baseret på Darcy's lov) og transportligningen (baseret på konvektions-dispersionsligningen) i tre dimensioner ved hjælp af finite difference metoder. For at kunne beskrive stofudbredelsen i opsprækkede bjergarter er modellen udbygget, således at vandfasen opdeles i en mobil del, som repræsenterer sprækkeporøsitet, og en ikke-mobil del, som repræsenterer matrixporøsitet. Transporten i et sådant system kan beskrives ved følgende differentialligning:

$$\theta_m \frac{\partial c_m}{\partial t} + \theta_{im} \frac{\partial c_{im}}{\partial t} = - \frac{\partial}{\partial x_k} (q_i c_m) + \theta_m \frac{\partial}{\partial x_i} \left(D_{ij} \frac{\partial c_m}{\partial x_j} \right) + S$$

$$\theta_{im} \frac{\partial c_{im}}{\partial t} = \beta (c_m - c_{im})$$

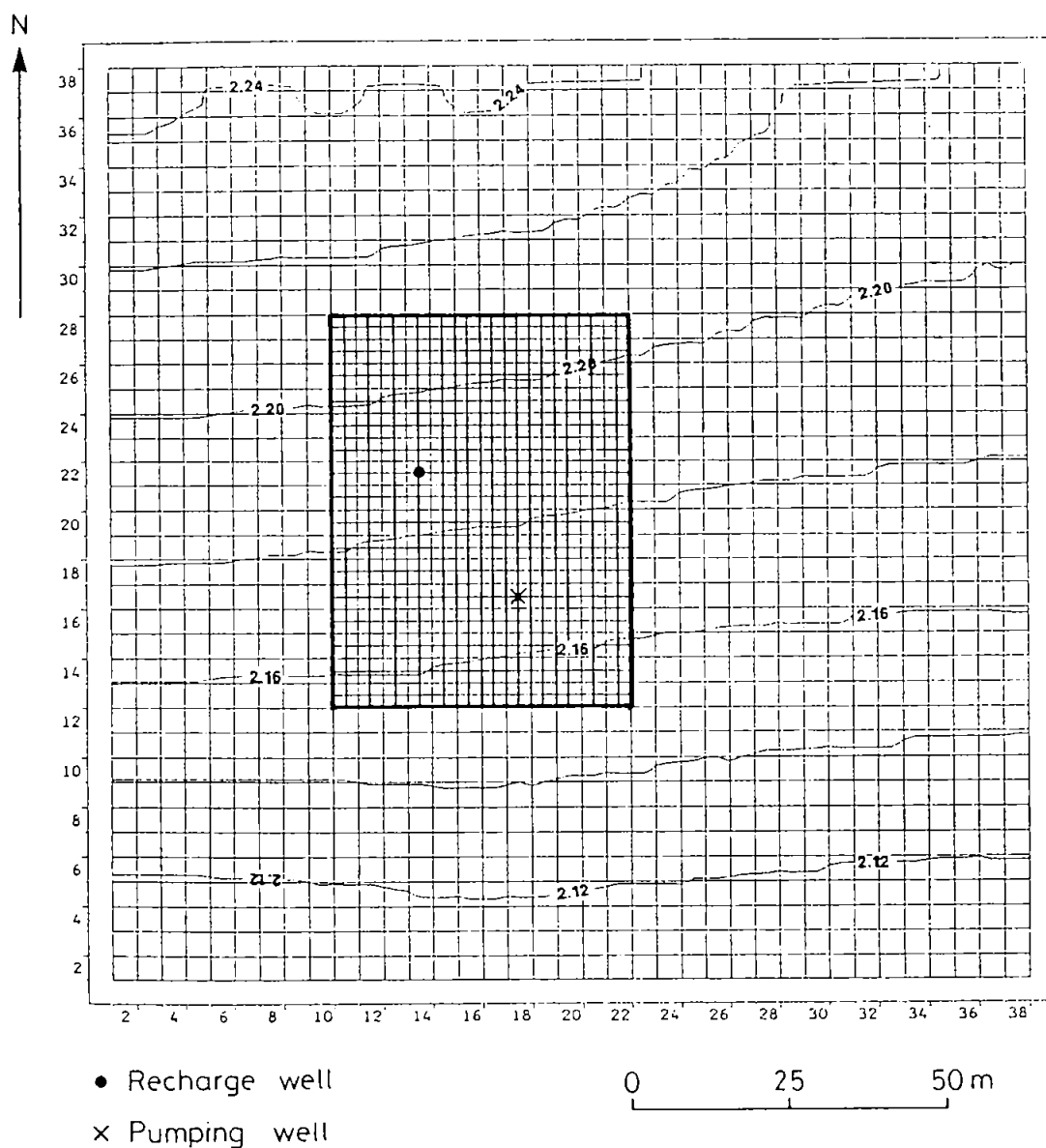
hvor

- c_m - koncentration i sprækker (mobil fase)
- c_{im} - koncentration i matrix (ikke-mobil fase)
- θ_m - sprækkeporøsitet
- θ_{im} - matrixporøsitet
- q_i - Darcy hastighed
- D_{ij} - dispersionskoefficient
- β - diffusionskoefficient
- S - kilde/dræn led
- x - stedkoordinater
- t - tid

Ligningen er udledt under følgende forudsætninger:

- 1) Vandstrømning, konvektion og dispersion forekommer kun i sprækkesystemet
- 2) Porerne i matrix er vandfyldte til alle tidspunkter, og vandet er stillestående

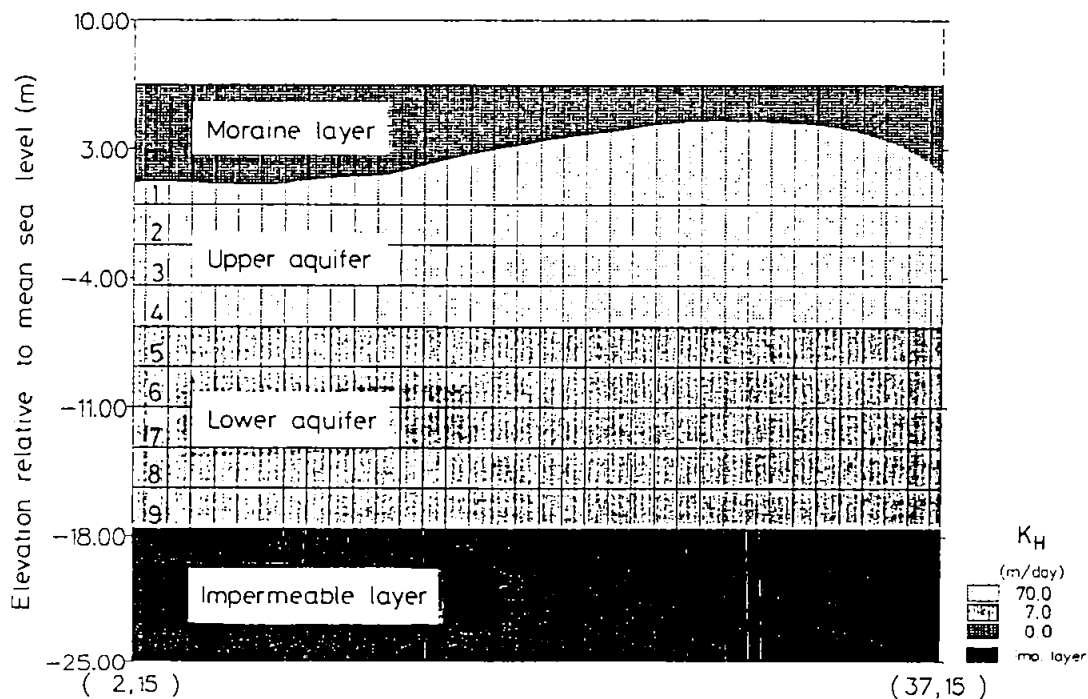
- 3) Forholdet mellem sprække- og matrixporøsiteterne ændrer sig ikke i tiden
- 4) Mellem sprækker og matrix foregår en stofudveksling ved diffusion.



Figur 3. Modelområde med horisontale diskretiseringer for vandstrømning (groft net) og stoftransport (fint net) samt simuleret potentialeforløb forud for sporstofforsøget.

Strømningsforholdene beskrives i et modelnet, som dækker et område på ca. 150 m × 150 m omkring forsøgsfeltet. Modelnettet er valgt, således at det er muligt at angive hensigtsmæssige vandbetingelser. Af hensyn til computertid simuleres stoftransport kun i et mindre område, Fig. 3.

Randbetingelser overføres automatisk fra det store område til delområdet. Strømningsmodellen indeholder $38 \times 38 \times 9$ numeriske elementer, som har en størrelse på 4 m × 4 m × 2.2 m, Fig. 6 og 7. I modelområdet for stoftransport anvendes en horisontal diskretisering på 2 m × 2 m.



Figur 4. Vertikal diskretisering og overordnet fordeling af hydraulisk ledningsevne.

Potentiallinierne antages at stå vinkelret på de vestlige og østlige rande (impermeable grænser), hvorimod fastholdte trykniveauer med hydrostatisk trykfordeling over dybden angives langs de nordlige og sydlige rande. Værdierne for hydraulisk trykniveau i de

enkelte beregningsselementer langs de to rande estimeres ud fra de foreliggende målinger i området.

Da forsøgsperioden er meget kort, er strømningsmodellen kalibreret under antagelse af, at de udførte potentialmålinger pr. 20.6.1990 repræsenterer en quasi-stationær situation. Videre antages, at der ikke forekommer nedsivning på dette tidspunkt.

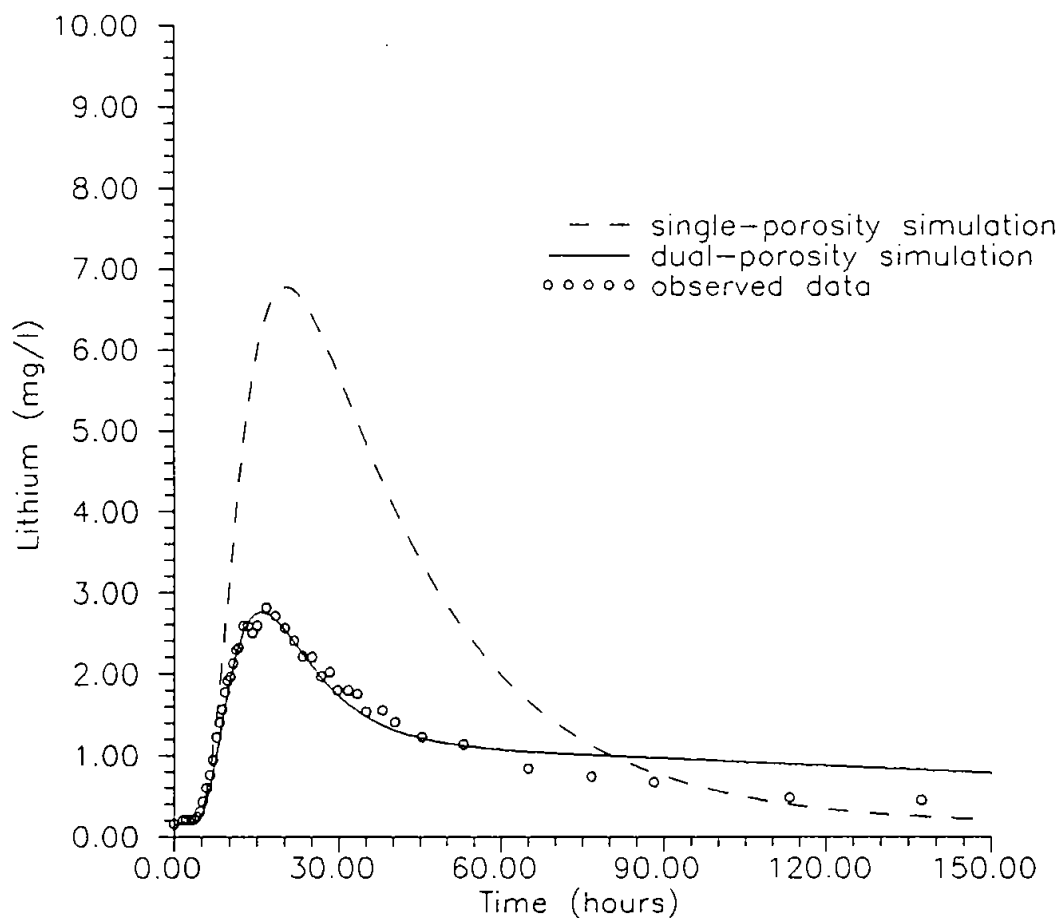
Feltundersøgelserne dokumenterede, at sprækkesystemet er mere udbygget i de øverste 10 m af kalkreservoiret. Dette er genskabt i modellen ved at introducere en øvre 10 m dyb mere permeabel zone og en nedre mindre permeabel zone af ca. 9 m's udstrækning. Ovenpå kalken introduceres et tyndt morænelersdække, som giver anledning til artesiske forhold i et mindre delområde inden for undersøgelsesfeltet, og nedadtil begrænses reservoiret af et impermeabelt lag i ca kote -18.0 m, jvf. Fig. 4. De hydrauliske parametre, som er introduceret i den numeriske model er sammenstillet i Tabel 1.

Kote (m)	Numeriske lag	K_H (m/d)	K_V (m/d)	Magasintal frit	Magasintal artesiske
Øvre zone moræne til -6.6 m	4	70.00	1.00	0.016	0.001
Nedre zone -6.6 m til -18.0 m	5	7.00	0.14	0.016	0.001

Tabel 1. Hydrauliske parametre anvendt i den numeriske model.

I Fig. 3 er vist det simulerede potentialbillede, som er i god overensstemmelse med de foreliggende feltmålinger.

Det er ikke muligt at beskrive de observerede gennembrudskurver under anvendelse af en traditionel enkeltporøsitetsmodel, hvor stoftransport kun foregår i sprækkesystemet. Resultatet er for hurtige transporttider og for høje koncentrationer, Fig. 5.



Figur 5. Observerede og simulerede (enkelt og dobbeltporøsitiesmodeller) gennembrudskurver for lag 2 i den numeriske model.

Introduceres en dobbeltporøsitetsbeskrivelse i modellen, er det derimod muligt at opnå en god beskrivelse af de observerede koncentrationer. For sprækkeporøsiteten er anvendt en værdi, som er i overensstemmelse med målingerne (1.1%), hvorimod det er nødvendigt at angive en værdi for matrixporøsiteten, som er væsentligt mindre end de foreliggende målinger (4.0%). Den fysiske forklaring på dette forhold er, at kun en mindre del af matrixporøsiteten deltager aktivt i diffusionsudvekslingen mellem de to domæner. Diffusionskoefficienten β , som indgår i procesbeskrivelsen, er bestemt ved kalibrering.

Dispersivitesparametrene, som indgår i transportligningen, er ligeledes bestemt ved kalibrering. For den langsgående dispersivitet anvendes en værdi på 8 m, hvorimod de øvrige dispersivitetsparametre er kalibreret til meget små værdier. En langsgående dispersivitet på 8 m er stor i forhold til skalaen for forsøget (25 m) og i forhold til den værdi, som er identificeret ved tracerfeltet ved Vejen (ca. 50 cm). Den høje værdi må tilskrives de meget heterogene forhold i opsprækkede bjergarter, som giver en forøget spredningsmæssig effekt.

Der er foretaget en følsomhedsanalyse for de vigtigste parametre i modelbeskrivelsen. Denne analyse har afsløret, at modelresultaterne er meget følsomme overfor både sprække- og matrixporøsiteterne og i særdeleshed overfor de mere empiriske parametre: diffusionskoefficienten og dispersiviteten.

5. KONKLUSION

Tracerforsøget i et opsprækket kalkmagasin ved Karlstrup har dokumenteret en hurtig udbredelse af en mindre del af traceren gennem sprækkesystemet, men samtidig er der tale om en betydelig forsinkelse af den resterende del af den tilførte tracer.

Modelanalysen har vist, at stoftransporten ikke kan beskrives ved en traditionel konvektion- dispersionsmodel for porøse medier. Ved at opdele det totale porevolumen i en sprækkeporøsitet, hvor transporten sker som konvektion og dispersion, og en matrixporøsitet, hvor vandet er stillestående, og med mulighed for diffusion mellem de to domæner, er det muligt at opnå en god beskrivelse af det observerede transportforløb. For sprækkeporøsiteten er anvendt en værdi, som er i overensstemmelse med feltmålingerne. Derimod er det nødvendigt at introducere en værdi for matrixporøsiteten, som er væsentligt lavere end de foreliggende målinger, fordi kun en mindre del af matrix deltager aktivt i diffusionsudvekslingen, når der er tale om transportforløb med lille tidsskala.

Videre har forsøget vist, at stofudbredelsen foregår tre-dimensionalt, hvilket fører til, at tre-dimensionale numeriske modeller er påkrævet i forbindelse med beregninger af forureningstransport i kalkmagasiner.

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Two-Well Tracer Test and Numerical Transport Modelling in Fractured Chalk

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Abstract

A two-well tracer test was conducted in eastern Denmark, in which a short duration pulse of lithium chloride was injected into a recharge well and made to flow through a fractured chalk aquifer to a discharge well. The wells were 25 meters apart, and the concentration of lithium arriving at the discharge well was monitored at five vertical intervals in the well for a 21 day period. The observed breakthrough curves show a sharp breakthrough front, with an arrival time that is consistent with advective transport through the fractures in the chalk. The breakthrough curves also exhibit a long tail in the falling limb, suggesting the influence of a secondary transport mechanism such as adsorption or diffusion of lithium into the porous matrix. To better understand the transport processes involved, a three-dimensional finite-difference model for flow and transport was constructed on the basis of geological and hydraulic information. The model was developed as a dual-porosity continuum model in which advection was assumed to occur only in the fractures, and the water in the porous matrix was assumed to be static. The exchange of solute between the fractures (mobile phase) and the porous matrix (immobile phase) was assumed to occur as a diffusion process in response to the local concentration difference of solute between the two phases. Simulations from the

dual-porosity model correctly reproduced the shape of the observed breakthrough curves, although some portions of the tail were not accurately represented. The model was also applied as a single-porosity model in which no diffusion or adsorption of solute were assumed to occur. The simulations from the single-porosity model greatly overestimated the observed lithium concentrations, and showed very little tailing effect in the falling limb. The study shows that, based on the given tracer test, solute transport in a fractured chalk cannot be represented by a single-porosity approach, and, hence, when dealing with contaminant transport in such systems, both a fractured and a porous domain need to be considered.

Overview

Groundwater represents an extremely important resource in Denmark. It provides over 99% of Denmark's drinking water supply, in addition to satisfying a large percentage of rural water needs. Due to the continued generation of industrial, municipal, and agricultural wastes and their subsequent sub-surface or surface disposal, however, an increasing amount of the country's groundwater resources has been threatened by contamination. If groundwater is to continue to play an important role in the development of Denmark's water resource potential, the fate of contaminants in groundwater must be better understood.

In eastern Denmark the water supply is often provided from water stored in fractured chalk aquifers. In order to better understand transport processes in a fractured porous medium, two field tracer tests were conducted in a fractured chalk aquifer near the town

of Karlstrup. This report describes the results of the second tracer test conducted at Karlstrup and the subsequent numerical simulations, which were performed by the application of a three-dimensional numerical flow and transport model. The field tests were conducted as "two-well tests", in which a short duration pulse of lithium was introduced into a recharge well and measured at several vertical intervals in a nearby pumping well, without recirculation of the pumped water. The results of the second test are presented as the observed concentrations of lithium from the discharge well in the form of breakthrough curves, as well as the simulated breakthrough curves from the numerical model. It is emphasized that the application of a numerical flow and transport model is not for predictive purposes, but rather a tool for understanding flow and transport in fractured porous media.

Field Site Geology and Hydraulic Parameters

The Karlstrup field site is located near the eastern shore of the island of Zealand, approximately 35 kilometers south of Copenhagen, Denmark (Fig. 1). The entire region is underlain by a thick sequence of chalk interbedded with flint layers, which serves as the regional aquifer. At most locations the chalk is covered by a thin layer of moraine with interbedded sand lenses, which ranges from 0 to 5 meters in thickness at the study site. The test site is an area approximately 80 meters by 120 meters, and contains 10 wells which penetrate the aquifer to a depth of approximately -20 meters (all depths are relative to mean sea level). Fig. 2 shows the location of the wells and the observed head levels in the aquifer prior to the second test.

The geology at the test site has been characterized on the basis of observations made at a nearby chalk quarry, and on data which have been obtained from the wells. The aquifer extends downward from the base of the moraine, and appears to be fairly homogeneous over the test site. In the vertical sense, the aquifer may be characterized as two distinct vertical layers based on fracture density. The upper layer extends from the base of the moraine to approximately -5 to -7 meters, and it contains numerous closely spaced fractures that appear to be randomly oriented. The lower section of the aquifer is geologically similar to the upper section, but contains a much lower density of fractures. The average fracture porosity of the upper layer is approximately 1.5 percent, based on the results of two pump tests conducted at the site. The total aquifer porosity, determined from core analysis, varies between 20 and 35 percent.

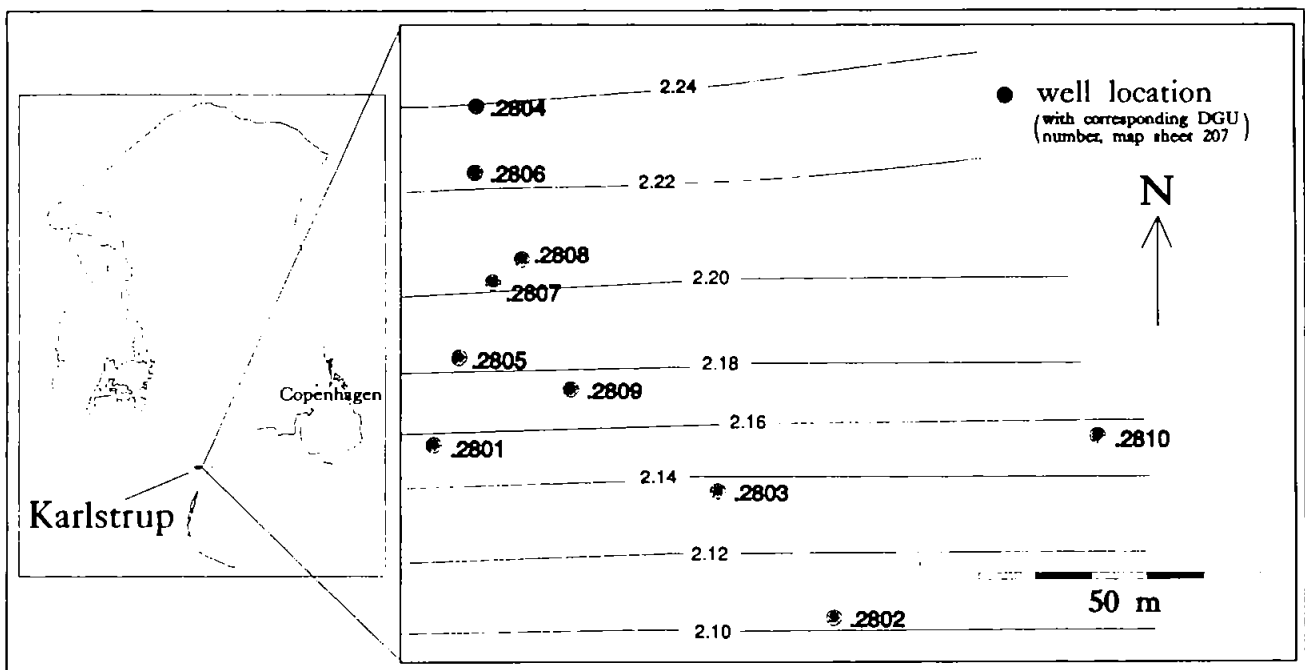


Figure 1. Location map of Karlstrup field site.

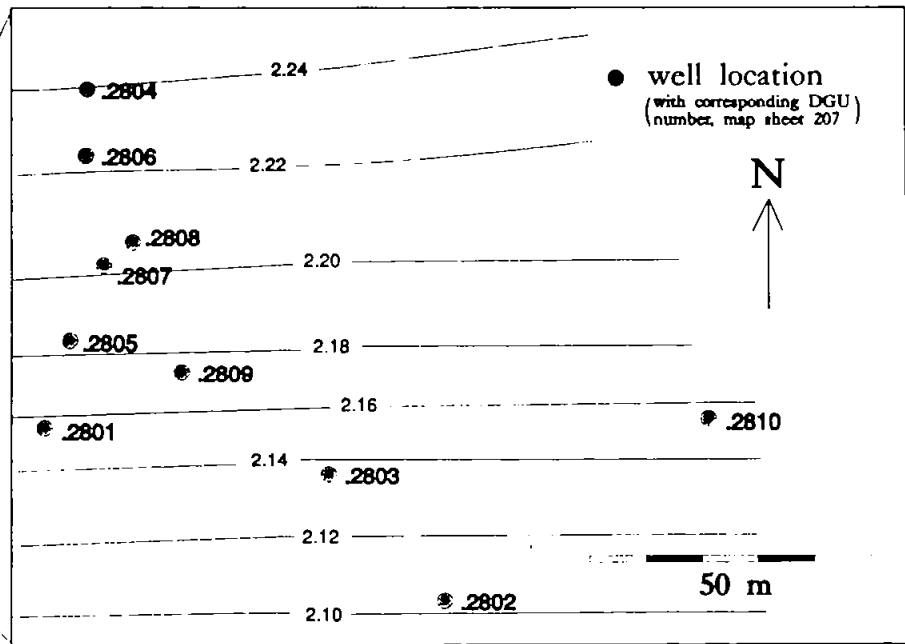


Figure 2. Plan view of well locations and the observed hydraulic head levels (m) prior to the second tracer test.

The hydraulic parameters of the aquifer have been determined based on the results of two pump tests, and a series of separation injection tests (SIT's) (Nilsson and Jakobsen, 1990) which were performed in each well in order to determine the vertical profile of horizontal hydraulic conductivity. During the SIT, fresh water and salt water are injected into the well bore simultaneously by two tubes located at the top and the bottom of the borehole, respectively (Fig. 3). A no-flow interface between the fresh water and the salt water is established in the borehole, the location of which is dependent on the ratio between the pumping rates and the hydraulic conductivity above and below the interface. By conducting the test multiple times while changing the ratio of the injection rates of the salt and fresh water in each test, the local horizontal hydraulic conductivity profile can be determined. Based on the results of the SIT's, the highest values of horizontal hydraulic conductivity are found in the upper 10 meters of the aquifer, corresponding to the region of highest fracture density. The horizontal hydraulic conductivity at this level of the aquifer is in the order of 50-100 m/day. According to the SIT's, approximately 90 percent of the flow occurs at this level of the aquifer. The lower interval of the aquifer is hydraulically tighter due to less extensive fracturing, and has a horizontal hydraulic conductivity of approximately 5 m/day. Analysis of the data from pump tests conducted at wells 2801 and 2807 (henceforth referred to as well 1 and well 7, respectively) indicates that the unconfined aquifer storativity is approximately .015, while the confined aquifer storativity is in the order of .001 - .005.

Groundwater flow occurs under unconfined conditions over most of the study site, with an average water table elevation of between 2 and 3 meters. Confined conditions exist over the southern one-third of the site where the water table extends into the overlying

moraine layer, which acts as a confining layer. Under natural flow conditions, a slight hydraulic gradient (.001) exists towards the south. Vertical head gradients within the aquifer appear to be small. Groundwater recharge is due to water infiltrating directly to the aquifer or through the overlying moraine.

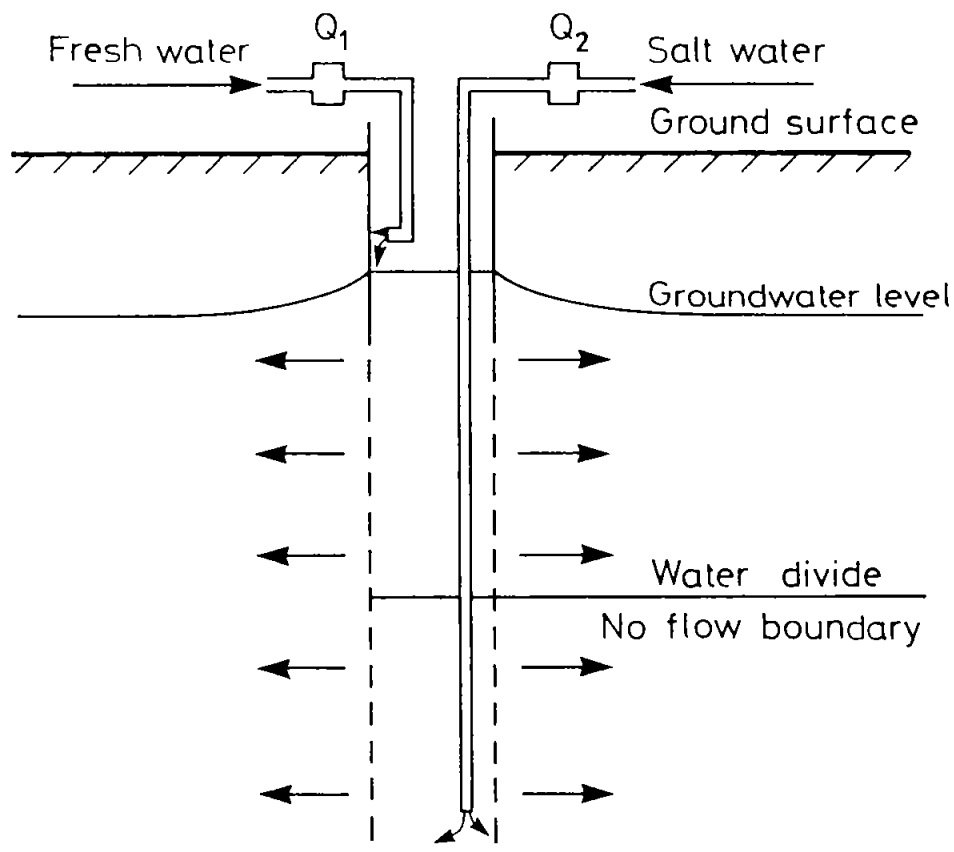


Figure 3. Schematic illustration of the separation injection test (from Nilsson and Jakobsen, 1990).

Literature Review

The transport of non-reactive solutes in groundwater is generally considered to be governed by two principal processes, advection and dispersion. Advection refers to the mean movement of solute in the flowing groundwater, while dispersion describes the spreading of solute about the mean motion caused by local variations of the groundwater velocity. Dispersion can be attributed to differences in hydraulic properties along the mean flow path.

The classical equation describing the transport of solutes in groundwater is the advection-dispersion equation, which can be written as:

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x_i} (v_i C) + \frac{\partial}{\partial x_i} \left(D_{ij} \frac{\partial C}{\partial x_j} \right) + S \quad (1)$$

where C is the concentration of the solute (M/L^3), D_{ij} is the dispersion coefficient (L^2/T), v_i is the pore-water velocity (L/T) equal to the Darcian flux q (L/T) divided by the volumetric water content θ (L^3/L^3), and S is a source/sink term. The above equation is valid for porous media that are fully saturated in which there is assumed to be no physical or chemical interaction between the fluid and the porous medium, and all of the fluid is assumed to participate in the flow process. However, for many soils and solutes, this is not the case. Solute may be adsorbed onto the soil, or part of the pore water may be stagnant and not participate in the flow process (Gaudet et al., 1977).

In a fractured porous medium, the total porosity may be divided into matrix porosity and fracture porosity. Matrix porosity generally refers to the inter-granular pore space due to grain size and sorting. Fracture porosity is usually due to a secondary process which can be mechanical, such as stress attributed to folding and faulting, or chemical, such as mineralogical alterations or solution channeling. Often the most rapid groundwater flow takes place in the fractures, which may only account for a small percentage of the overall porosity of the medium. The water stored in the porous matrix may account volumetrically for most of the water in the medium, but it may not significantly contribute to groundwater flow and can therefore be considered as "static" water (Gaudet et al., 1977; Bibby, 1981). In this situation the effective porosity, defined as the volume of interconnected void space contributing to flow per unit bulk volume of rock, may be much lower than the actual porosity of the medium (Gordon, 1986). Although the water in the porous matrix may not significantly contribute to groundwater flow, it may still play an important role in transport processes by acting as a long-term natural reservoir for solute retention (Lawrence et al., 1990). In such situations, the controlling influences on the transport of solutes may not be convection and dispersion, but, rather, secondary processes such as adsorption, reaction, and diffusion of solute into static water (Bibby, 1981).

In many ways the effect of static water on mass transport is similar to the effects produced by solute diffusion into dead-end pores and solute adsorption onto the solids of the porous medium (Bibby, 1981). Solute exchange by diffusion can occur between the fractures and the porous matrix at a rate that may depend on several factors, such as the difference in solute concentration between the fracture water and the pore water, and

the length of the diffusion paths. This diffusion can significantly attenuate solute concentrations in the fractures (Lawrence et al., 1990), as well as increase the retention time of solute in the aquifer. The diffusion of solute from the static water to the fractures, which occurs when the solute concentration in the fractures declines below the solute concentration in the porous matrix, can also considerably affect solute transport. In this situation, the porous matrix acts as a source of solute to the fractures, sometimes long after the original solute source has been eliminated.

In developing a transport model for fractured media, the central issue is whether to model the system as an equivalent porous medium (continuum) or as a discrete fracture network (noncontinuum) (Van Rooy, 1987). The continuum approach is often desirable, since flow and transport models that have been developed for granular porous media can be applied. The continuum approach may not always be valid, however, in which case the fracture system must be described either deterministically or stochastically. Stochastic approaches aim to characterize the fracture properties by probability density functions, which requires statistical information to describe the fracture parameters. Such information may be difficult to obtain when applying a field scale model.

In order to assess the validity of the continuum approach, Long et al. (1982) used theoretical aspects of flow through fractured media to determine when a fractured rock behaves as a continuum. Among their criteria for using the continuum approach, they determined that there should be an insignificant change in the value of the equivalent permeability of the medium for small changes in the sample size, and that fracture systems behave more like equivalent porous media as the fracture density is increased.

Such criteria are difficult to apply, since they only address the problem qualitatively.

Of the groundwater models that address transport in fractured media, most treat the aquifer as an equivalent porous medium. Numerous continuum models appear in the literature, for example van Genuchten and Wierenga (1976), Grisak and Pickens (1980), and Bibby (1981). Transport models which treat the aquifer as a discrete fracture system are less common, and have usually only been used in an experimental mode. Smith and Schwartz (1984), for example, used a stochastic modelling technique to investigate mass transport within a network of discrete fractures in which fracture length, location, and aperture were characterized by probability distributions.

In addition to modelling fluid flow in the fractures, many groundwater transport models have a component which accounts for the transfer of solute between the fractures, or mobile phase, and the pore water, or immobile phase. Of the dead-end pore models that are described in the literature, most have been developed for the continuum type of transport model. Many of these dead-end pore models assume that the immobile water in the pores is in intimate contact with the mobile water phase (Coats and Smith, 1964; Gaudet et al., 1977; van Genuchten and Wierenga, 1976). These models assume that the diffusion paths are very short, allowing the process to be described by a linear equation. One of the classic linear dead-end pore models is described by Coats and Smith (1964):

$$\frac{\partial C_s}{\partial t} = \frac{k}{n_s}(C_n - C_s) \quad (2)$$

where C_s and C_n describe the solute concentrations in the immobile and mobile water

phases, respectively, n_s is the porosity of the porous matrix, and k is the diffusion mass transfer coefficient.

Other models have been developed in which the mobile and immobile phases are assumed not to be in intimate contact, resulting in a non-linear diffusion process. Bibby (1981) developed an analytical solution for diffusion in a fractured chalk aquifer in England that was characterized by relatively large, highly porous blocks of chalk which were separated by narrow fissures. Using an analytical solution for diffusion of a finite mass from a fissure into a porous block, he showed that it may be many days before the rate of mass transfer reduces to an approximately linear form. The model, however, gives rise to a large number of calibration parameters, which requires an extensive amount of data from the aquifer, which are normally not available.

Field Tracer Test

During the summer of 1990, two tracer tests were conducted by the Geological Survey of Denmark at the Karlstrup field site in order to investigate transport processes in a fractured chalk aquifer typical of eastern Denmark. The tests were conducted as "two-well tests" in which a short duration pulse of lithium chloride was made to flow from an interval of several meters in a recharge well to a discharge well over a horizontal distance of approximately 25 meters. The concentration of lithium arriving at the discharge well was monitored in the discharge water from five pumps which were placed at various vertical locations in the well. Although two tracer tests were conducted, this report will focus on the results of the second test.

The second tracer test at Karlstrup began on August 2, 1990 when the five pumps that had been installed in well 2809 (the discharge well, henceforth referred to as well 9) were started and pumped at $1.2 \text{ m}^3/\text{hr}$ (total discharge from the well was $6.0 \text{ m}^3/\text{hr}$). There were no packers present in the well, so the pumps were assumed to withdraw water from the surrounding chalk based on the 20 percent flow partials established from the separation injection test in well 9. After the well had been pumped for approximately 7 hours, the tracer injection began at well 7, which was located 25 meters from well 9 (see Fig. 2). The injection began with fresh water being pumped into the well from two tubes that were positioned at the top and the bottom of the well bore, respectively. Fresh water was pumped into the upper interval at $1.2 \text{ m}^3/\text{hr}$ and into the bottom interval at $3.6 \text{ m}^3/\text{hr}$. After 10 minutes of fresh water injection, the injection of a lithium chloride solution commenced from a tank containing 944 mg/l of lithium. The lithium solution was injected into the well at a rate of $1.2 \text{ m}^3/\text{hr}$ from an additional tube located in the well bore at -2 meters. The lithium solution was pumped into the well for 53.5 minutes, such that the total mass of lithium injected was 1010 grams. After the lithium had been injected, fresh water continued to be injected above and below the tracer interval for another 30 minutes in order to flush any remaining lithium from the well bore. The injection of fresh water above and below the interval of tracer injection was also intended to isolate the lithium to a relatively narrow interval in the well bore, since no packers were present in the well. A certain amount of mixing occurred in the well bore nevertheless, such that lithium was injected into the formation over the vertical extent of the well at varying concentrations. Lithium concentrations were monitored at five intervals in the recharge well during and after the tracer injection in order to characterize the vertical distribution of lithium in the well bore. The discharge well was pumped at

a steady rate throughout the 21 day duration of the test, and water samples were taken from the outflow of the five pumps and analyzed for lithium.

Observed Lithium Movement

In order to describe the transport of lithium between the recharge well and the discharge well, lithium concentrations were monitored in the pumped water from the five flow partials identified by the SIT tests. Breakthrough curves were obtained by plotting the observed lithium concentrations vs. time for these intervals (Fig. 4). Examination of the breakthrough curves shows that the highest observed peak concentrations of lithium are found in the interval from 0 to -2 meters, corresponding to the interval where most of the lithium mass was injected in well 7. Lower peak concentrations of lithium were observed above and below this interval, especially just below the aquifer-moraine interface and also in the deepest intervals of the aquifer where relatively low concentrations of lithium were found in the recharge well. This suggests that the lithium migration was not affected by any major density contrasts. The breakthrough curves are quite asymmetrical, as they exhibit a sharp breakthrough front followed by a long tail which gradually approaches the background lithium concentration of .16 mg/l. The presence of this tail suggests that the lithium transport was affected by some process(es) in addition to advection and dispersion in the fractures.

It is also interesting to note that the arrival times of the peak lithium concentrations in the discharge well were approximately the same for all the intervals (about 17 hours after lithium injection began), with the exception of the uppermost interval where the arrival

time of the peak was about 24 hours. For the deepest interval this is somewhat surprising, because the hydraulic conductivity at the lower level of the aquifer is at least one order of magnitude smaller than it is in the upper aquifer. One possibility is that the relatively lower fracture porosity in the lower interval compensates for the low value of hydraulic conductivity, resulting in groundwater velocities that are the same order of magnitude as those found in the upper aquifer. Another possible, and perhaps plausible, way to describe this observation is to assume that the lithium detected in the bottom interval of the discharge well actually was transported through the higher conductivity layers of the upper aquifer. Upon reaching the discharge well, this lithium could have mixed into the lowest interval of the well and therefore been discharged through the lowermost pump in the well. This seems quite possible considering that no packers were present in the discharge well to restrict mixing in the borehole, and the lowermost pump was located approximately one to two meters below the interval where the highest concentrations of lithium were measured.

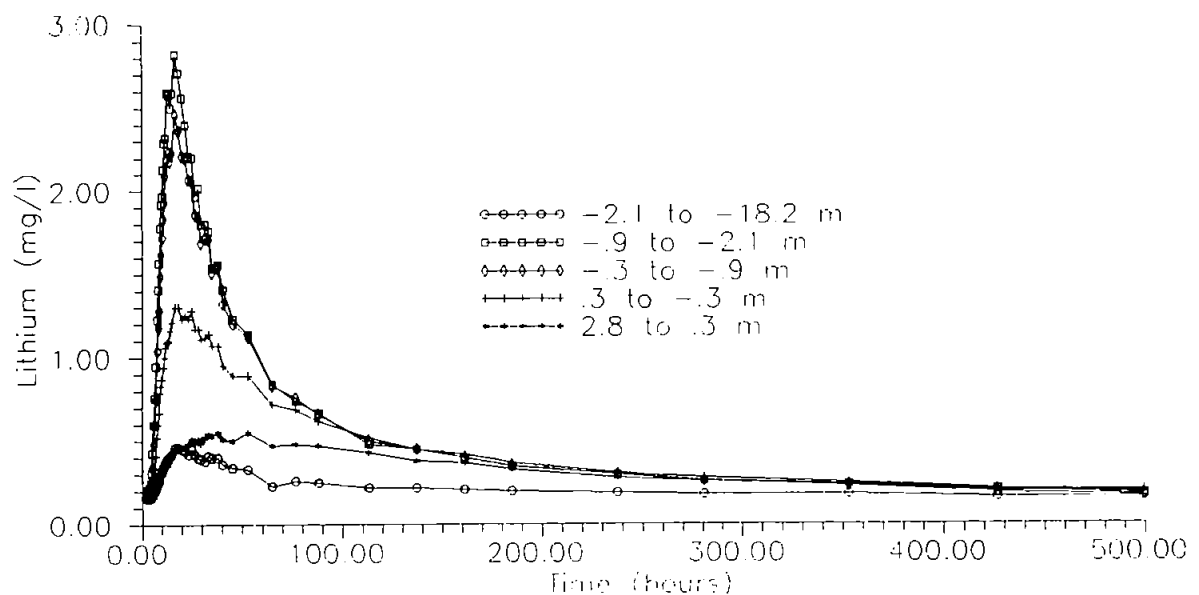


Figure 4. Observed breakthrough curves of lithium from five vertical intervals in the discharge well.

Numerical Model

In order to analyze lithium transport in the aquifer over specific vertical intervals, a three-dimensional flow and transport model was constructed based on geological and hydraulic information. The model used was the saturated zone module from the European Hydrological System (SHE), which is a finite-difference model based on the governing differential equations for flow and transport in a saturated, porous medium (Ammentorp and Refsgaard, 1990). In the case of a fractured porous medium, flow and advective transport are assumed to occur only in the fractures. The water in the porous matrix is assumed to be static, such that the porous matrix has no influence on groundwater flow but does affect solute transport by participating in the molecular diffusion of solute between phases.

Groundwater flow in the fractures is based on the governing equation for three-dimensional Darcy-type flow based on a continuum approach:

$$S \frac{\partial h}{\partial t} = \frac{\partial}{\partial x_i} \left(K_{ij} \frac{\partial h}{\partial x_j} \right) - R \quad (3)$$

where:

h	-	hydraulic head
K	-	hydraulic conductivity
S	-	specific storage
R	-	source/sink term

The transport of solutes in the saturated zone is described by solving a form of the advection-dispersion equation which includes a term accounting for the diffusion of solutes between the fractures (mobile phase) and the porous matrix (immobile phase):

$$\theta_m \frac{\partial C_m}{\partial t} + \theta_{im} \frac{\partial C_{im}}{\partial t} = -\frac{\partial}{\partial x_i} (q_i C_m) + \theta_m \frac{\partial}{\partial x_i} \left(D_{ij} \frac{\partial C_m}{\partial x_j} \right) + S \quad (4)$$

where:

- C_m - solute concentration in the mobile phase
- C_{im} - solute concentration in the immobile phase
- θ_m - fracture porosity (mobile phase)
- θ_{im} - matrix porosity (immobile phase)
- q_i - Darcy flux
- D_{ij} - dispersion coefficient
- S - source/sink term

The dispersion coefficient is related to the groundwater velocity using Scheidegger's (1961) equation:

$$D_{ij} = \alpha_{ijmn} \frac{u_m u_n}{|u|} \quad i, j, m, n = 1, 2, 3 \quad (5)$$

where:

- α - dispersivity
- u - seepage velocity
- $|u|$ - magnitude of seepage velocity

In order to simplify the dispersion description, only the diagonal terms of the dispersion tensor are considered. Due to symmetry and for physical reasons, four components of the dispersivity tensor are defined: α_{LH} (longitudinal horizontal dispersivity), α_{LV} (longitudinal vertical dispersivity), α_{TH} (transverse horizontal dispersivity), and α_{TV} (transverse vertical dispersivity).

The exchange of mass between the mobile and the immobile water phase as a result of molecular diffusion is included in the model as a distributed source/sink term. The adopted approach assumes that the mobile and the immobile waters are in intimate contact, and that the diffusion paths are short, and can be described mathematically by:

$$\theta_{im} \frac{\partial C_{im}}{\partial t} = \beta (C_m - C_{im}) \quad (6)$$

where β is the diffusion mass transfer coefficient. This model compares favourably with the experimental data of Coats and Smith (1964), and has been used by others to model solute diffusion between two phases (Gaudet et al., 1977; van Genuchten and Wierenga, 1976).

Model Application

To solve the flow and transport equations numerically, a finite-difference grid was developed to represent the model area. In order to minimize the effects of the model boundaries, the flow equation was initially solved over a rectangular-shaped grid that was 152 meters on a side, with a horizontal node spacing of 4 meters. The grid was oriented such that boundary conditions along the vertical planes bordering the model region were either prescribed head boundaries or no-flow boundaries, depending on orientation (Fig. 5). The east-west trending boundaries were essentially perpendicular to the natural hydraulic head gradient, and were treated as fixed head boundaries assuming that hydrostatic conditions applied. The north-south trending boundaries were parallel to the natural flow lines and were considered no-flow boundaries. Since a finer numerical discretization was desired for transport modelling, a finer grid was developed to cover the immediate test area (Fig. 5). This grid was 48 by 64 meters, and had a horizontal node spacing of 2 meters. The boundary conditions used for the fine grid simulation were obtained from the coarse grid solution.

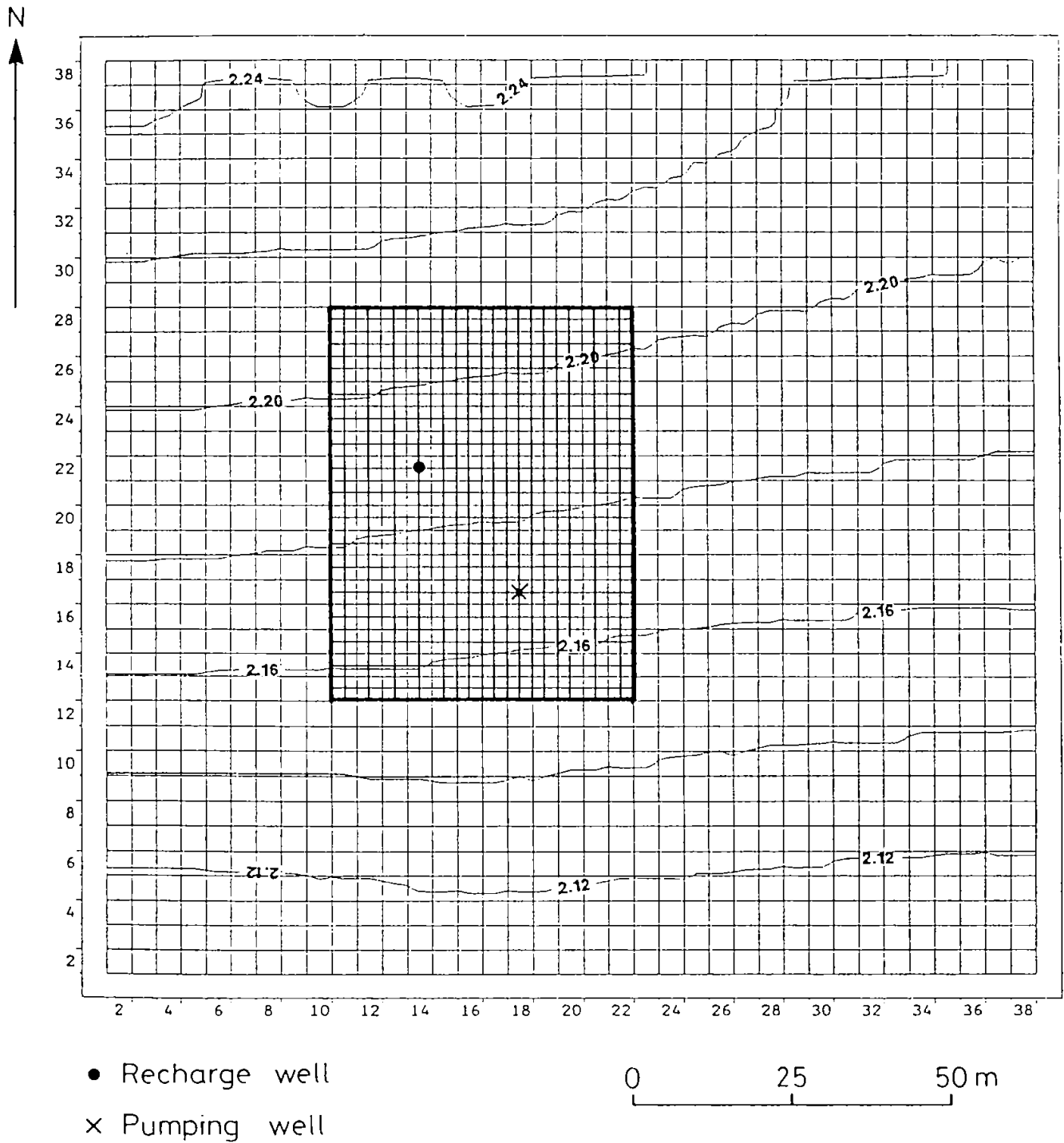


Figure 5. Horizontal discretization in the numerical model (coarse grid), with the outlined region showing the area over which lithium transport was simulated (fine grid). Hydraulic head values (m) represent simulated conditions prior to the second tracer test.

In the vertical plane, the aquifer was represented by nine numerical layers, each with a thickness of 2.2 meters (Fig. 6). The upper four layers corresponded to the highly fractured section of the aquifer, and were modelled using a horizontal hydraulic conductivity of 70 m/day. The lower five layers represented the less permeable section of the aquifer, in which a horizontal hydraulic conductivity of 7 m/day was used. The bottom boundary was treated as a no-flow boundary, since very little flow appears to occur in the aquifer below this depth. An additional layer was used in the model to represent the moraine layer. Since the moraine layer has a low permeability, no flow or transport were assumed to occur in this layer and therefore the aquifer-moraine interface was modelled as a no-flow boundary. Aquifer recharge normally occurs from the vertically downward movement of water through the moraine, but was assumed to be negligible over the short duration of the given test. A timestep of 15 minutes was used for both the flow and transport modelling, which was selected in order to accurately simulate the non-steady nature of the tracer injection.

Simulation Results

In order to define the groundwater velocity field over the region of the tracer test, flow simulation was performed first over the coarse numerical grid and subsequently over the fine numerical grid. The pumping and injection rates used in the model were based on the actual rates used during the field test, while the initial values of hydraulic conductivity and storativity were based on calculated values from the SIT's and the two pump tests. Calibration of the flow models was an iterative process which was performed by matching simulated head levels to the observed head levels in the observation wells. Since most

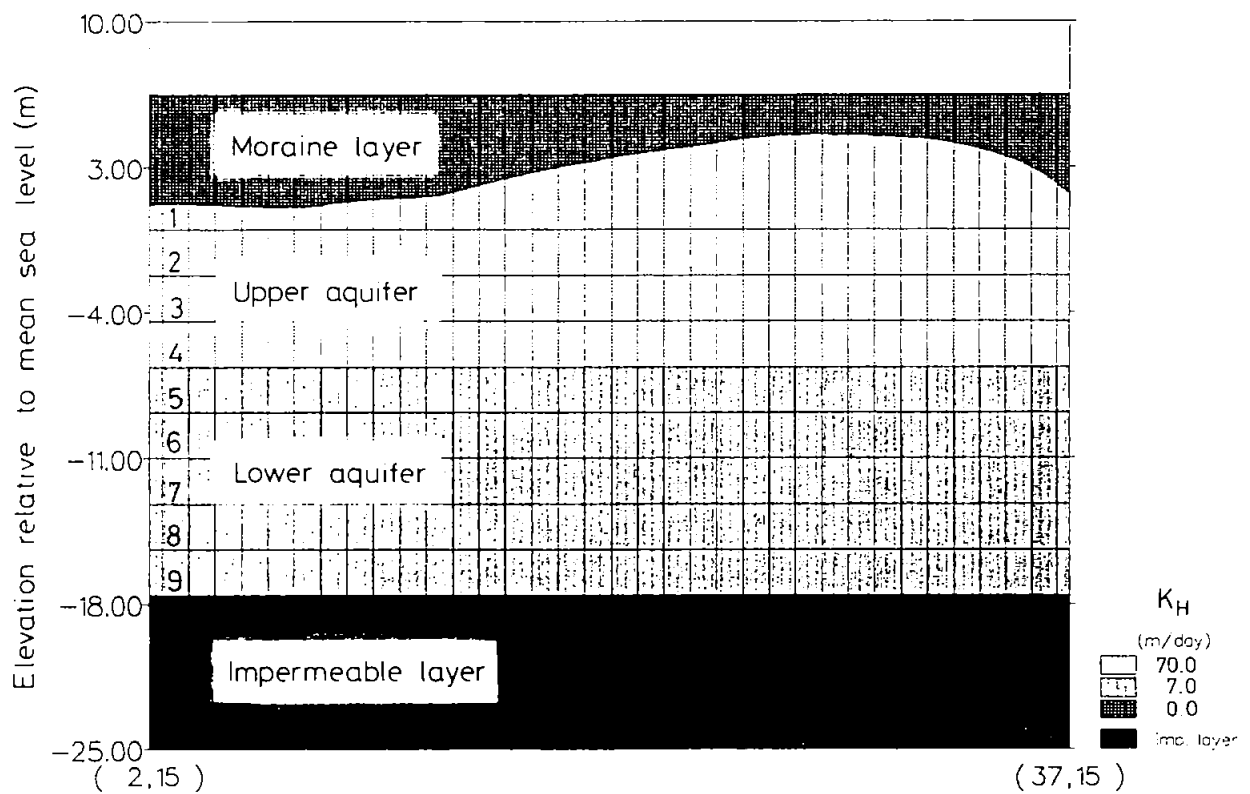


Figure 6. Vertical discretization of the aquifer in the numerical model.

of the lithium transport occurred between wells 7 and 9, it was most important to properly define the velocity field in this region. It was difficult to accurately reproduce the observed head values in all of the wells, so emphasis was placed on reproducing the observed head gradients between the recharge well and the discharge well. Calibration showed that the flow model was most sensitive to the horizontal hydraulic conductivity, although both hydraulic conductivity and storativity were adjusted to achieve a satisfactory calibration of the model. The calibration of the flow model was complicated by the sensitivity of the transport model to the definition of the velocity field between the recharge well and the discharge well. For the final calibration it was necessary to

"iterate" between the flow and transport models in order to achieve a satisfactory calibration of the transport model. The flow model was used to calculate the development in the velocity field over the fine grid for the first 30 hours of the tracer test, after which a steady state velocity field was assumed. This was justified by the small changes in hydraulic head which were observed after 30 hours of pumping. Figures 7 and 8 show the simulated head levels in the aquifer over the fine numerical grid during and after the lithium injection, respectively.

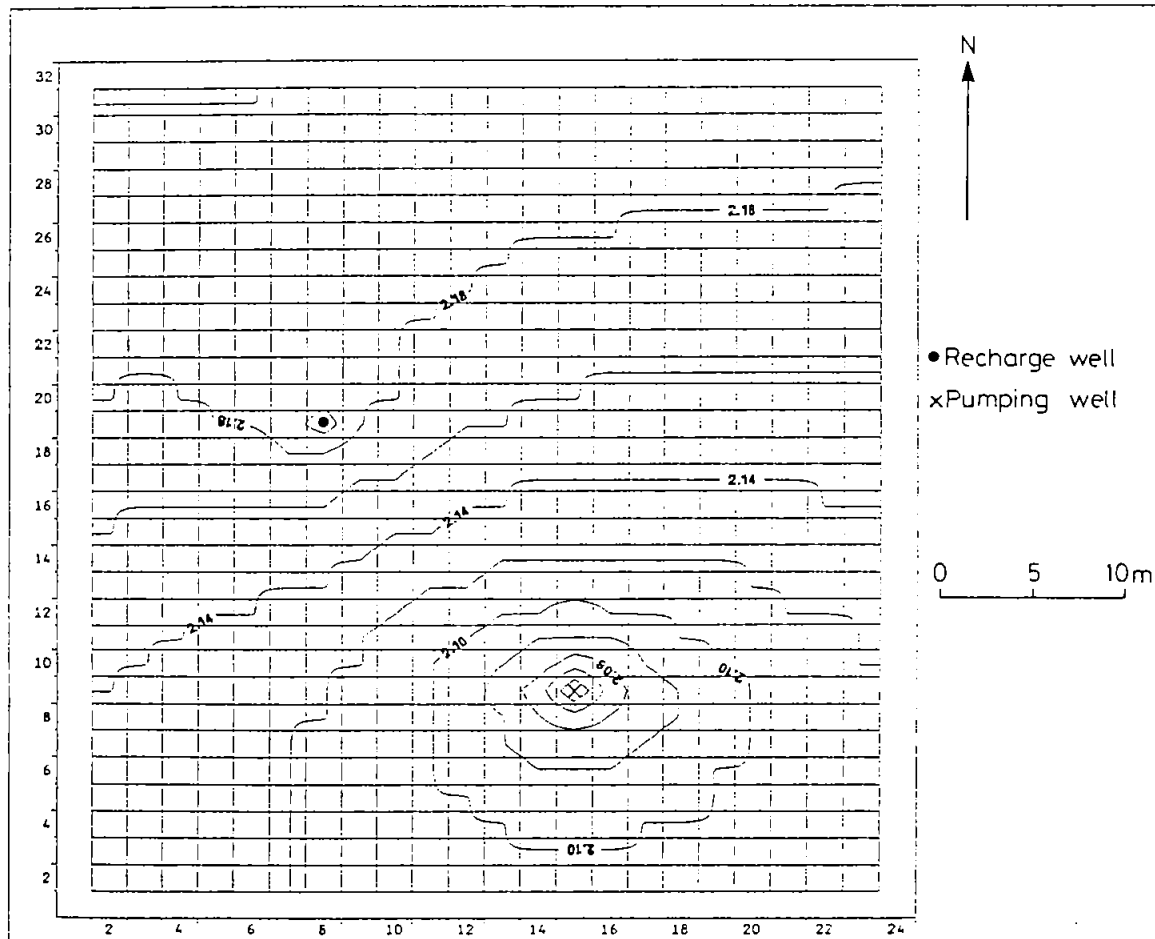


Figure 7. Simulated hydraulic head levels (m) over the fine finite-difference grid during lithium injection ($t=7$ hours).

The transport model was also based on the assumption that the aquifer was composed of two homogeneous layers. Although lithium was detected over the vertical extension of both the recharge and the discharge wells during the test, lithium transport was assumed to occur only through the upper aquifer, based on the assumption that lithium detected in the lowermost interval of the discharge well was transported through the upper interval of the aquifer. As a result, lithium was applied in the numerical model only to the upper aquifer. Based on measured lithium concentrations in the injection well from an electric conductivity sonde, 70 percent of the lithium was assumed to enter the aquifer in the interval corresponding to layers 3 and 4 in the numerical model. The remaining 30 percent was applied to layers 1 and 2 in the numerical model. Although it was difficult to accurately know the vertical distribution of lithium that was input to the aquifer, the injection rates, length of injection, and total mass of lithium applied in the model represent the actual values from the field test.

For the purpose of determining the appropriate hydraulic parameters to use in the model, it was assumed that the horizontal hydraulic conductivity in the upper aquifer was 10 times greater than it was in the lower aquifer. This assumption was based on data that were obtained from the separation injection tests. In addition, it was assumed (somewhat arbitrarily) that vertical hydraulic conductivities throughout the aquifer were at least 50 times smaller than the horizontal values. Values for specific storage were used in the model depending on whether confined or unconfined conditions existed and were selected based on data obtained from the pump tests. The hydraulic parameters that were used in the simulations are listed in Table 1.

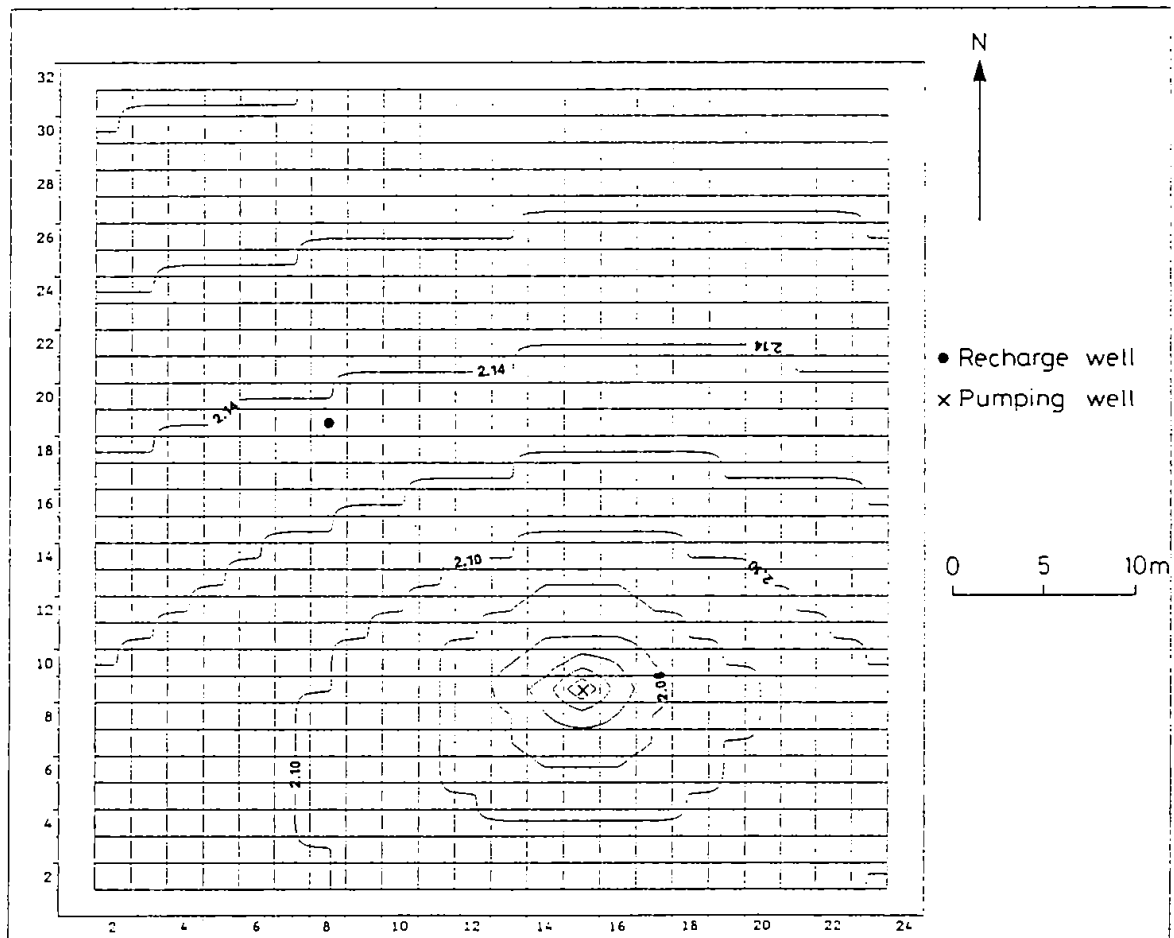


Figure 8. Simulated hydraulic head levels (m) over the fine finite-difference grid at steady state conditions (t=30 hours).

Aquifer level (metres)	Numerical layers	K_H (m/d)	K_V (m/d)	unconfined storativity	confined storativity
Upper moraine base to -6.6 m	4	70.00	1.00	0.016	0.001
Lower -6.6 m to - 18.0 m	5	7.00	0.14	0.016	0.001

Table 1. Hydraulic parameters used in the numerical simulations to represent the aquifer.

The transport model was originally developed as a single-porosity model, in which transport was assumed to occur only in the fractures due to advection and dispersion. Using a single-porosity approach, all attempts to match the simulated breakthrough curves to the observed data were unsuccessful. In all cases the simulated results greatly overestimated the observed lithium concentrations, and were unable to reproduce the long tailing effect observed in the data (Figs. 9,10,11). By assuming that lithium transport occurred only in the fractures, the entire mass of injected lithium moved through the aquifer too rapidly, such that 100 percent of the injected mass was recovered at the discharge well after only 6 days (144 hours). According to lithium measurements at the discharge well, however, only 47 percent of the lithium had been recovered after 6 days (see Fig. 12). After a sharp breakthrough front of the rising limb and peak concentration, the observed breakthrough curves exhibit a long tail of relatively low lithium concentrations which was present throughout the remainder of the test, indicating that some mechanism was retarding the flow of lithium between the wells. This tailing effect was perhaps even more pronounced in the upper intervals of the aquifer, as shown in Figs. 10 and 11.

Subsequent modelling was based on a dual-porosity approach, in which the porous matrix was represented in the model as a reservoir for solute retention. The exchange of solute between the fractures and the porous matrix was assumed to occur by diffusion in response to local differences in solute concentration between these two phases. The initial simulations that were conducted with the dual-porosity model used parameter values that were based on the observed values for the fracture and matrix porosity, while the dispersivities were taken from the values used in the single-porosity model. The coefficient, β , which controls the rate of solute diffusion between the two phases, has little physical meaning and was therefore used purely as a calibration coefficient. In order to determine the "best-fit" parameters for the model, the simulated breakthrough curve obtained from layers 3 and 4 of the model (an average breakthrough curve from these two layers) was fitted to an observed breakthrough curve corresponding to the same vertical interval of the aquifer. By adjusting the values for porosity, longitudinal horizontal dispersivity, and β , simulated breakthrough curves were produced which satisfactorily reproduced the observed breakthrough curves from the upper interval of the

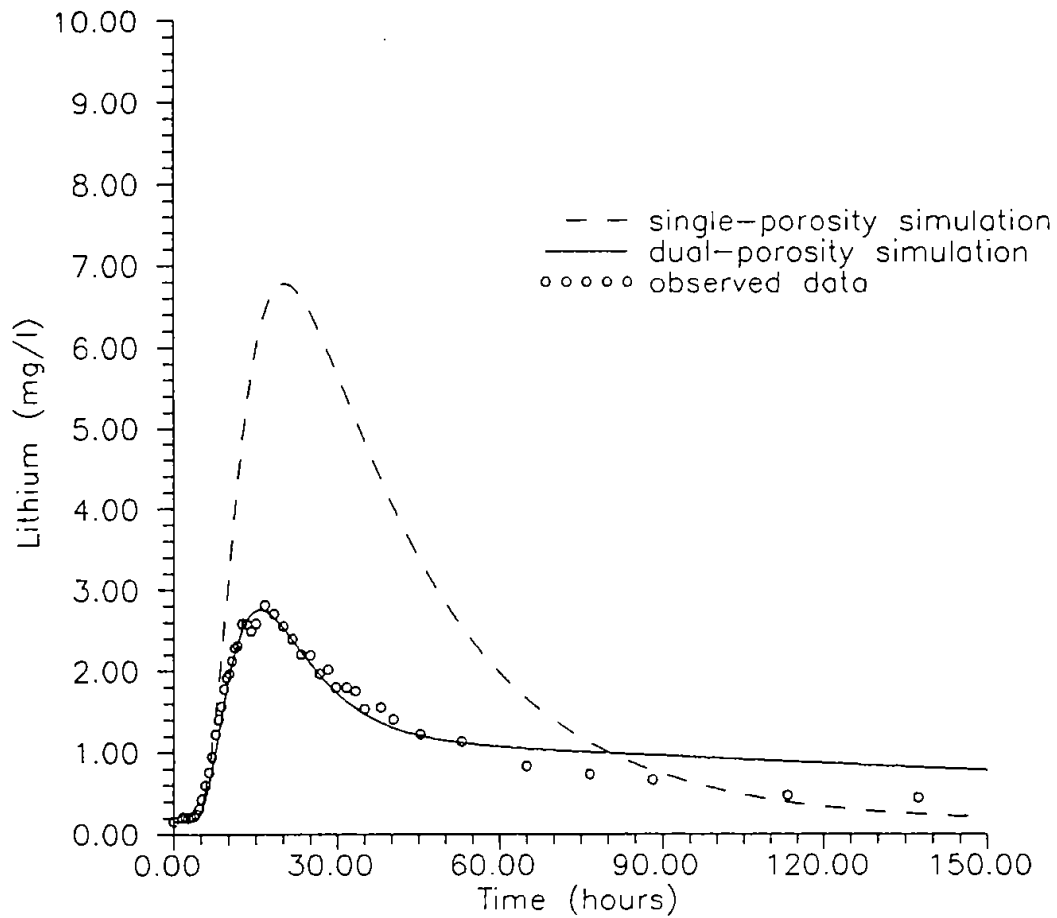


Figure 9. Comparison of simulated breakthrough curves from the single and dual-porosity models to observed lithium concentrations at the discharge well. The simulated curves correspond to the average output from layers 3 and 4 of the numerical model.

aquifer (see Figs. 9,10, and 11). For the three intervals that were simulated, the peak concentration and the overall shape of the curves were reproduced quite well, although some portions of the tail were not represented well in each of the intervals. The simulated breakthrough curves obtained from layers 1 and 2 of the model (Figs. 10 and 11) were not used in the calibration process, so they are presented mostly as a validation of the model calibration.

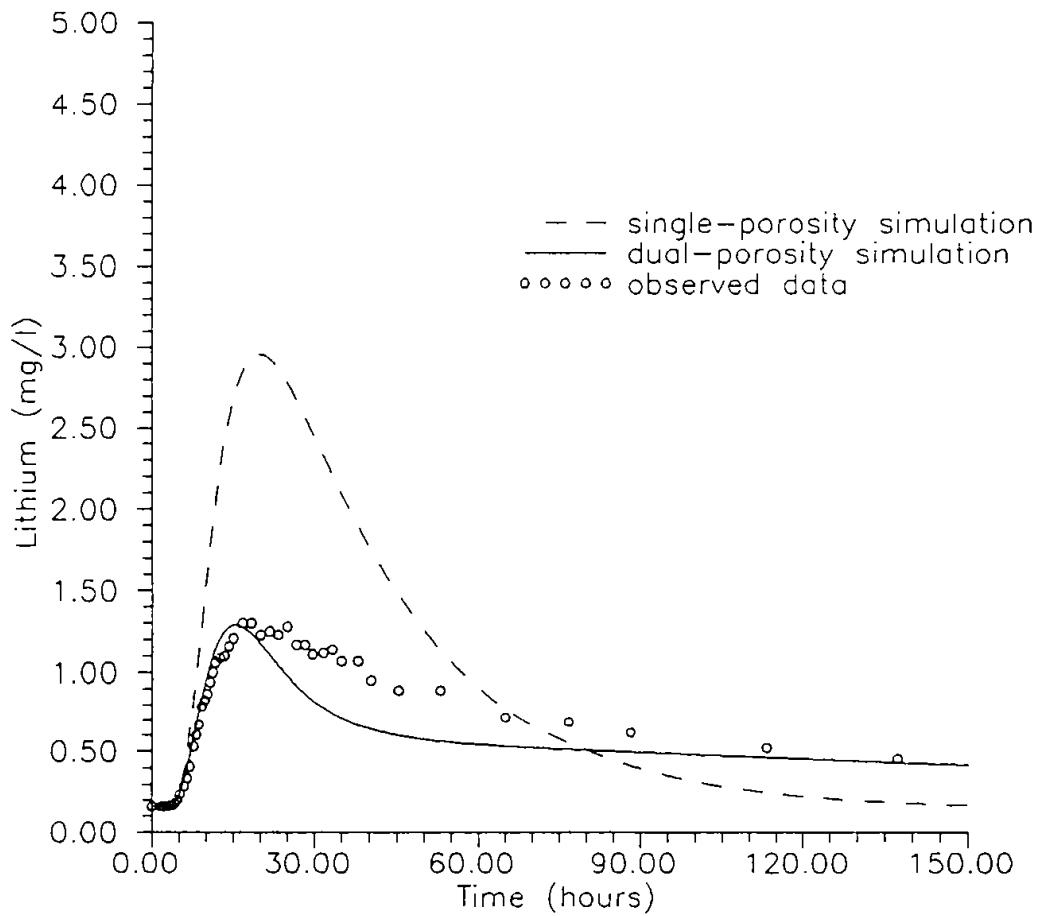


Figure 10. Comparison of simulated breakthrough curves from the single and the dual-porosity models to observed lithium concentrations at the discharge well. The simulated curves correspond to the output from layer 2 of the numerical model.

Based on the given calibration technique, a set of best-fit parameters were obtained for the dual-porosity transport model. Although some of the calibrated parameters are mostly empirical coefficients with little physical meaning, others such as the porosity values can be measured directly from the aquifer. For instance, the fracture porosity, which was calibrated to 1.1 percent in the model, was reasonably close to the spatially averaged value of 1.5 percent determined from the pump tests. Since advective transport was assumed to occur only in the fractures, the magnitude and the arrival time of the peak concentration were quite sensitive to this parameter, as shown in the results of a

sensitivity analysis (Fig. 13). Decreasing the fracture porosity causes a proportionate increase in the groundwater velocities in the fractures, resulting in an earlier breakthrough of the peak concentration. The peak concentration will be higher as a result of a smaller fracture porosity, mainly because less solute dilution will occur in the fractures. Increasing the fracture porosity will have the opposite effect: slower overall travel times and lower peak concentrations.

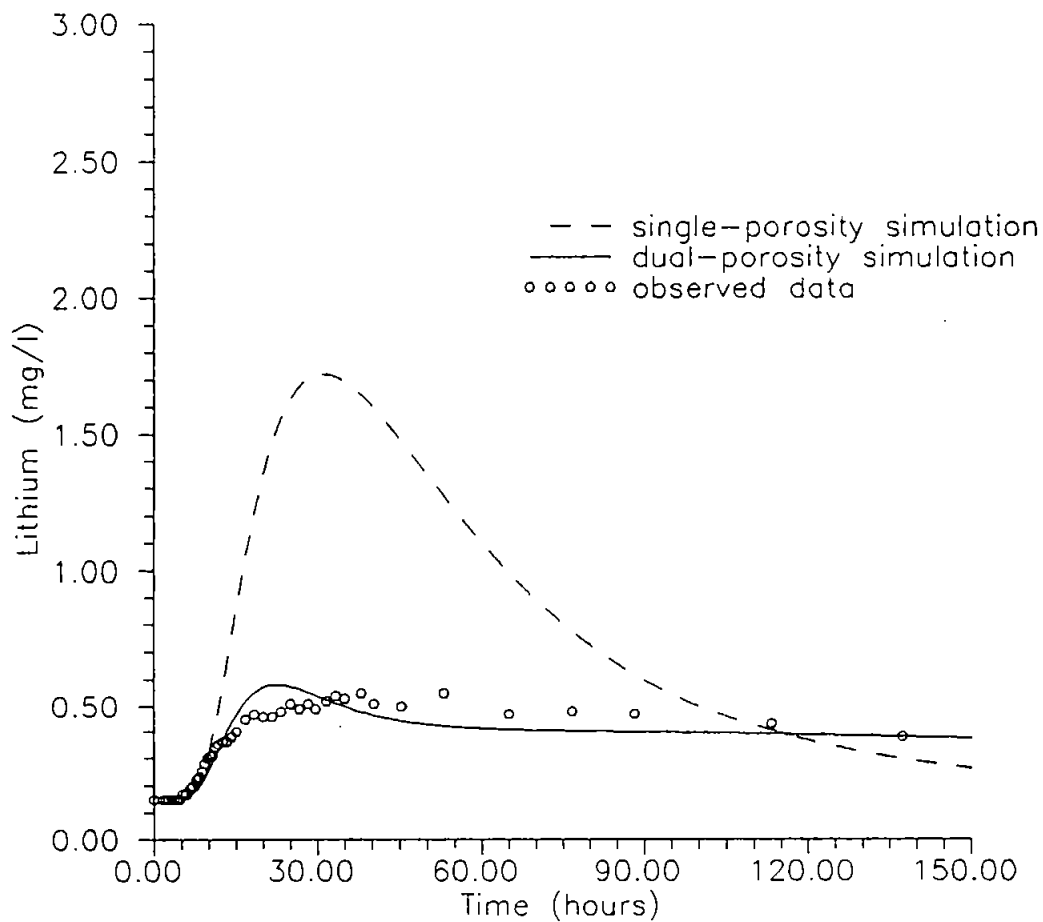


Figure 11. Comparison of simulated breakthrough curves from the single and the dual-porosity models to observed lithium concentrations at the discharge well. The simulated curves correspond to the output from layer 1 of the numerical model.

The sensitivity of the dual-porosity model to the matrix porosity was also investigated (Fig. 14). It is evident that the model is most sensitive to this parameter at low values. The matrix porosity appeared to have no effect on the initial breakthrough front, although it had a slight effect on the peak breakthrough concentration and a significant effect on the tail of the breakthrough curve. As the amount of matrix porosity that is involved in solute exchange becomes greater, a larger amount of solute will initially diffuse to the matrix in an attempt to achieve solute equilibrium between the phases. This will result in more of the solute being stored in the matrix, such that the tail following the initial breakthrough pulse will have a relatively low concentration but will continue for a long duration as the solute slowly diffuses back to the fractures. Conversely, as the matrix porosity becomes smaller, less solute will diffuse to the matrix in an attempt to achieve solute equilibrium. In this case more of the solute will pass through the fractures with the initial pulse, resulting in breakthrough curves with higher overall concentrations but shorter duration tails.

As seen from the sensitivity analysis, the calibrated value for the matrix porosity was 4 percent, which is significantly lower than the values suggested by core analysis (20-35 percent). The physical significance of such a small matrix porosity can be justified, however, if one considers that this value does not necessarily represent the entire matrix porosity, but rather the matrix porosity that is actively involved in solute diffusion. Considering the short duration of the test, it seems reasonable that only a fraction of the total matrix porosity was involved in the diffusion process. This would most likely represent the pores that are in closest contact with the fractures. Unfortunately, it was not possible to confirm this hypothesis with field or laboratory measurements, so the physical validity of this value remains unclear.

The dispersivity values that were used in the initial simulations were based partly on the calculated dispersivities for a fractured chalk at Dorset, England that are reported in a review by Gelhar et al. (1985). A sensitivity analysis was subsequently conducted in order to identify the dispersivity values which most closely reproduced the observed breakthrough curves. Based on this analysis, the simulated breakthrough curves appear to be quite sensitive to the longitudinal horizontal dispersivity (Fig. 15). Since this

parameter controls how much the lithium plume will spread, it is an important parameter for determining when the initial breakthrough of lithium will occur. The peak concentration of the breakthrough curve is also sensitive to this parameter, especially to small values of α_{LH} .

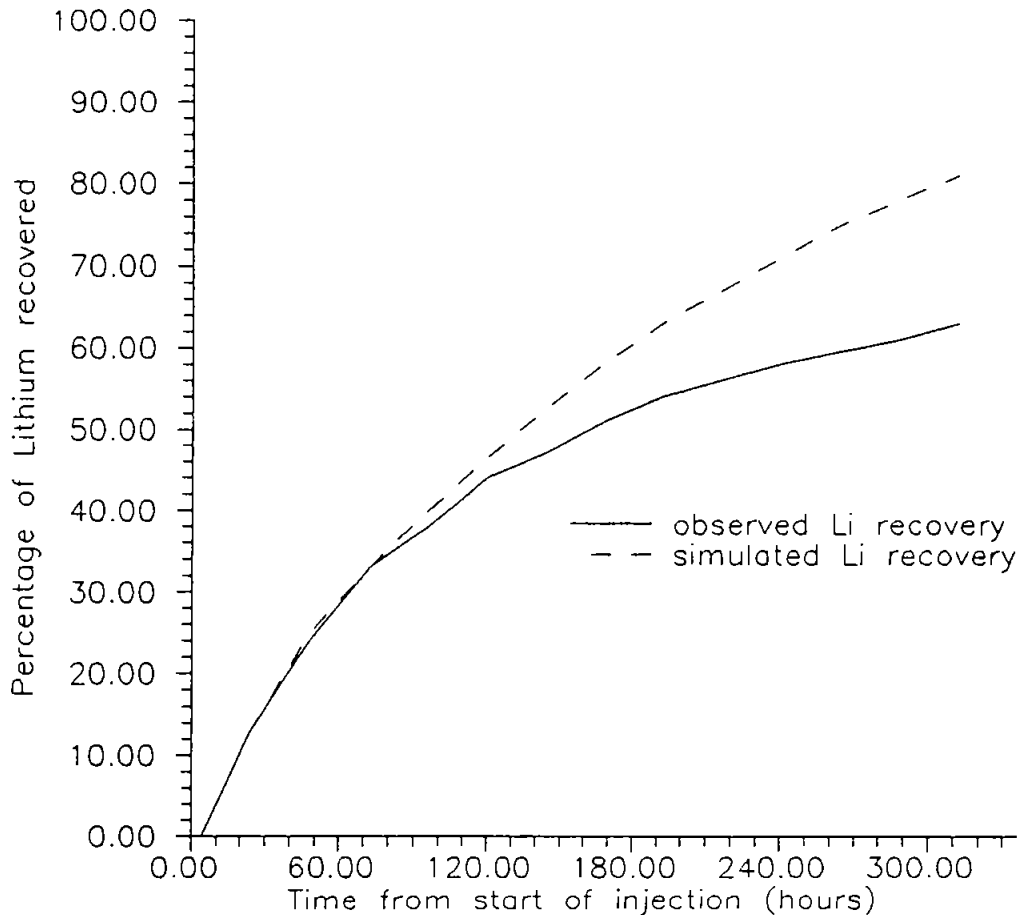


Figure 12. Comparison of the simulated and the observed percentage of injected lithium recovered at the discharge well vs. time.

The dispersivities in the vertical direction had virtually no effect on the simulation results due to insignificant vertical flow components. During the calibration of the transport model, the dispersivities in the horizontal direction were adjusted in order to help fit the peak and the rising limb of the simulated breakthrough curve to the observed data. On

the basis of calibration, the "best-fit" dispersivities were determined to be: $\alpha_{LH} = 8.0\text{m}$, $\alpha_{TH} = 0.05\text{m}$, $\alpha_{LV} = 0.001\text{m}$, and $\alpha_{TV} = 0.001\text{m}$.

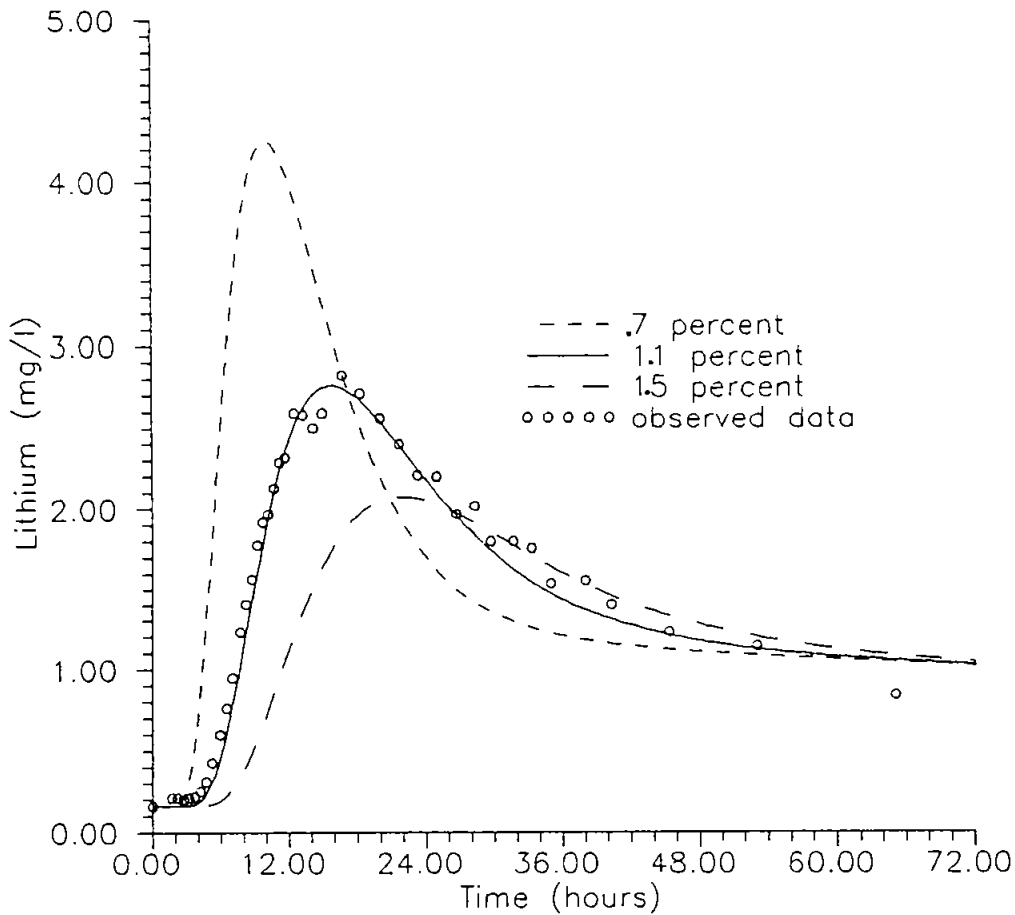


Figure 13. Sensitivity of the simulated breakthrough curve (layers 3 and 4) from the dual-porosity model to the fracture porosity of the aquifer.

The longitudinal horizontal dispersivity, α_{LH} , appears to be quite high, especially at the scale of the test (25 meters). Although this value compares reasonably well with the dispersivities reported from a similar test (Gelhar et al., 1985), a report by Welty and Gelhar (1989) suggests that many previous interpretations of longitudinal dispersivity from breakthrough curves tend to overestimate the value of this parameter. While it is likely that the reported "best-fit" dispersivities may be rather high, Gordon (1986) has concluded that a substantial amount of dispersion can arise from the heterogeneity of a

discontinuously-fractured medium. Perhaps the heterogeneity introduced by the random fracture orientation in the chalk at least partly accounts for the large value of α_{LH} .

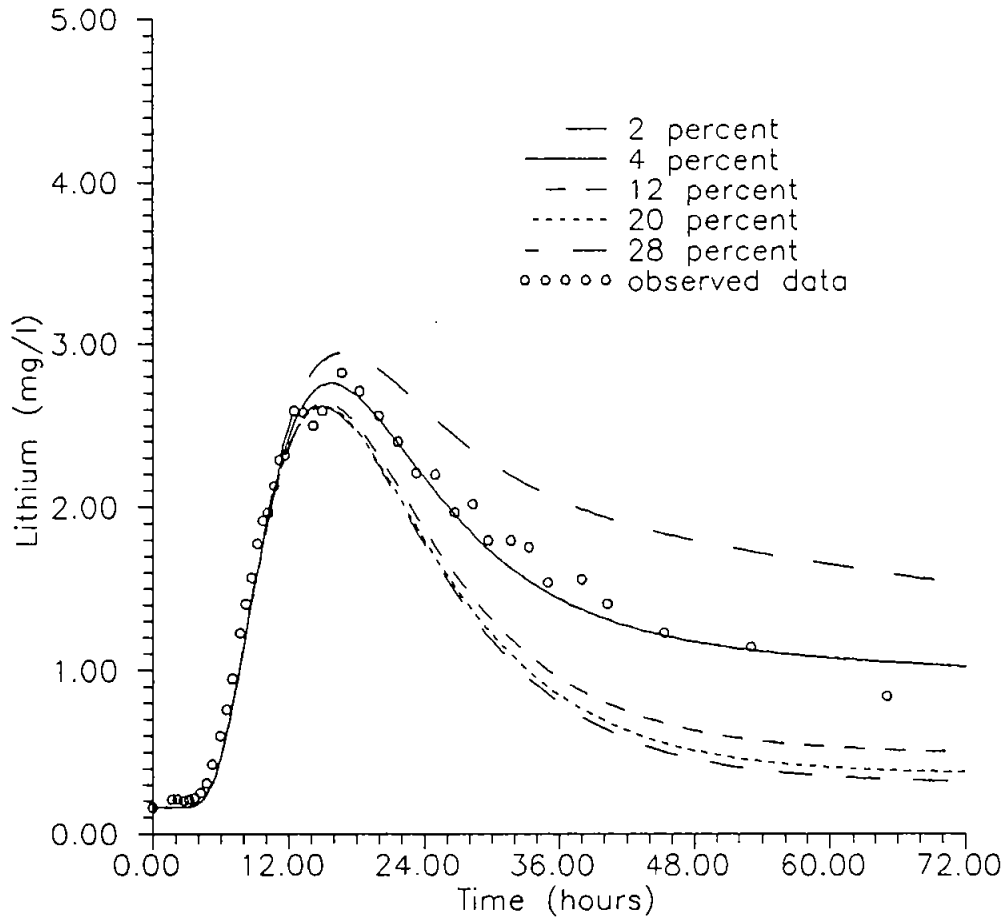


Figure 14. Sensitivity of the simulated breakthrough curve (layers 3 and 4) from the dual-porosity model to the matrix porosity which is actively involved in solute diffusion.

The diffusion mass transfer coefficient, β , is an empirical parameter which was determined to have an optimal value of $2.0e-07$ based on curve-fitting. As shown in Fig. 16, the simulated breakthrough curves are very sensitive to this parameter, since it controls the rate of solute exchange between the mobile and the immobile water phases. As β is increased, solute diffusion takes place at a faster rate, which causes a more rapid attenuation of the peak solute concentrations in the fractures. The effect is to shift more of the solute mass to the tail of the breakthrough curve, such that a relatively long

duration tail of high concentration is obtained. Decreasing β decreases the rate of diffusion, which diminishes the effect that solute diffusion has on the overall transport process for a short-duration tracer test.

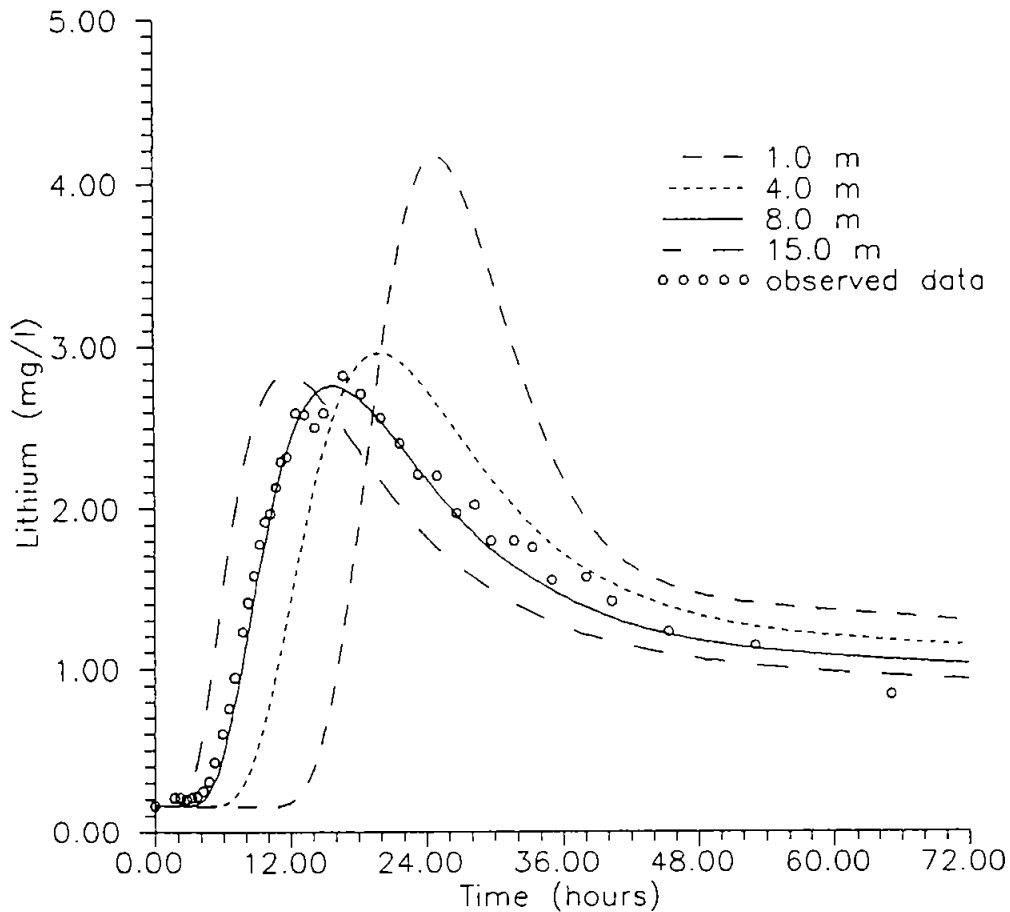


Figure 15. Sensitivity of the simulated breakthrough curve (layers 3 and 4) from the dual-porosity model to the longitudinal horizontal dispersivity, α_{LH} .

In order to understand better the mechanisms involved in lithium transport through the aquifer, a comparison can be made between the simulated breakthrough curves and the observed data (Figs. 9, 10, and 11). Based on the results of the simulations, it is quite evident that the lithium mass moves through the aquifer at a much slower rate when it is transported according to a dual-porosity model, which is consistent with the observed data. The main effect of lithium diffusion into the porous matrix is to retard the

transport of lithium through the aquifer. In the dual-porosity model, the slow movement of lithium through the aquifer can be explained by an initially rapid diffusive exchange of lithium between the fractures and the porous matrix, and the subsequent retention of this lithium in the matrix. According to simulation from the dual-porosity model, most of the lithium was transferred to the porous matrix shortly after injection, such that 81 percent of the lithium remaining in the aquifer after 2 days was stored in the matrix. This lithium remained in the matrix until the concentration gradient was favourable for lithium to diffuse from the matrix to the fractures. Since the reversal of the concentration gradient can be a slow process, solute can be held in the matrix for a long time, such that the matrix behaves as a long-term source of solute to the fractures which at least partly explains the observed tailing effect on the breakthrough curves.

Another mechanism which quite possibly affects lithium transport is the adsorption of lithium onto the aquifer material. Lithium has been shown to be a reactive tracer in other field tests, one of the best examples being the Cape Cod tracer test (LeBlanc et al., 1991) in which lithium transport was shown to be retarded when compared with the non-reactive tracer, bromide. Laboratory experiments by Wood et al. (1990) suggest that for the Cape Cod study, the majority of the reaction sites for lithium were in grain interiors, such that most reactions were preceded by lithium diffusion into the aquifer material. The study by LeBlanc et al. (1991) also suggests that although lithium may be acting as a reactive substance, this effect is not seen immediately. A comparison of the movement of bromide and lithium at the Cape Cod site showed that as late as 33 days after the tracer injection, there was little difference in the areal distribution of the two plumes. This seems to suggest that the reaction of lithium was not a significant factor during the earlier stages of the test. Since the Karlstrup test lasted only 21 days, it seems possible that if lithium was being adsorbed onto the chalk, any adsorption effects would have been overshadowed by the initial diffusion of lithium into the matrix. Adsorption might have been somewhat more significant during the later stages of the tracer test, and it could partly account for more lithium remaining in the aquifer than was calculated by the dual-porosity model (see Fig. 12).

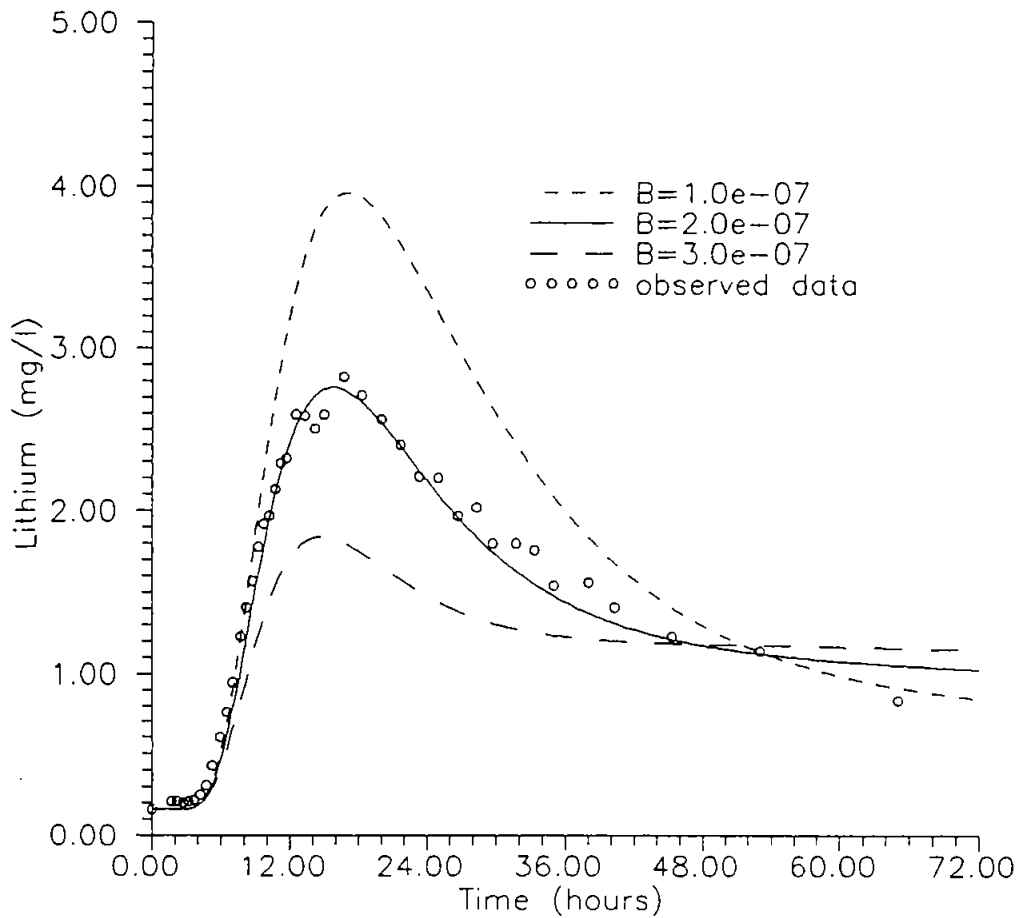


Figure 16. Sensitivity of the simulated breakthrough curve (layers 3 and 4) from the dual-porosity model to the diffusion mass transfer coefficient, β .

Summary and Conclusions

A two-well tracer test using lithium chloride was conducted in a fractured chalk aquifer as a means to investigate solute transport in a fractured porous medium. To better understand the transport processes involved, a numerical flow and transport model was constructed to simulate the field test. The model was originally applied using a single-porosity continuum approach, but was later modified to a dual-porosity continuum model to simulate solute diffusion between the fractures and the porous matrix. Solute diffusion

was assumed to occur as a linear process in response to the local concentration differences of solute between the two phases.

The parameter values used in the models were based on measured hydraulic parameters as well as calibrated values that were obtained by fitting simulated breakthrough curves to the observed data. The simulations using the single-porosity model greatly overestimated the observed lithium concentrations, and were unable to reproduce the long tail observed on the falling limb of the observed breakthrough curves. Simulations using a dual-porosity approach, on the other hand, correctly reproduced the shape of the observed breakthrough curves, although some portions of the tail were not accurately represented. A sensitivity analysis was subsequently conducted in order to determine the sensitivity of the model to selected parameters.

Based on the observed data and the simulated results, it is apparent that solute transport in a fractured chalk cannot be represented by a single-porosity approach. Although most of the groundwater flow and hence advective transport may take place in the fractures, mass transport appears to be controlled, at least initially, by the molecular diffusion of solute between the fractures and the essentially static water in the porous matrix. Depending on the amount of matrix porosity that is actively involved in the diffusion process, a significant amount of solute can diffuse to the porous matrix and remain in storage until the local concentration gradient favours reverse diffusion back to the fractures. This process can significantly attenuate the peak solute concentrations in the fractures, as well as greatly increase the retention time of solute in the aquifer.

The simulated results also suggest that only a portion of the total matrix porosity may be actively involved in solute diffusion, although no field measurements have been made to confirm this. The most favourable simulation results were obtained using a matrix porosity of 4 percent, which is considerably lower than the values of 20 to 35 percent that were determined by core analysis. Based on the relatively short time scale of the given test, it seems possible that only the pores in closest contact with the fractures participated in the diffusive exchange of solute.

Another mechanism which may affect lithium transport is the adsorption of lithium ions onto the aquifer material. Although adsorption was not considered in the present study, past field tests have shown lithium to be a reactive tracer. It is likely that adsorption may have been an important process during the later stages of the Karlstrup test, although solute diffusion appears to be the dominant process during the earlier stages of the test. It is evident that larger-scale field investigations involving conservative and non-conservative tracers are needed in the future in order to consider the effects of solute reaction in a fractured chalk. The present study does, however, show that when dealing with contaminant transport in a fractured medium, both a fractured and a porous domain need to be considered.

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